STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 180215

TO: Nyeemah Grazier **Location: REM-5B29&5C18** **Art Unit: 1626** **March 10, 2006** **Case Serial Number: 10/765267**	**From: P. Sheppard** **Location: Remsen Building** **Phone: (571) 272-2529** **sheppard@uspto.gov**

Search Notes

ACCESS DB # 80215

FOR OFFICIAL USE ONLY

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Paula

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Nyeemah Grazier Examiner #: 81002 Date: 2/22/06

Art Unit: 1626 Phone Number: 2-8781 Serial Number: 10/765,767

Location (Bldg/Room#): Rem 5B29 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK

****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Methods, Mixtures & Kits Pertaining to Analyte Determinabi

Inventors (please provide full names): Pappin et al.

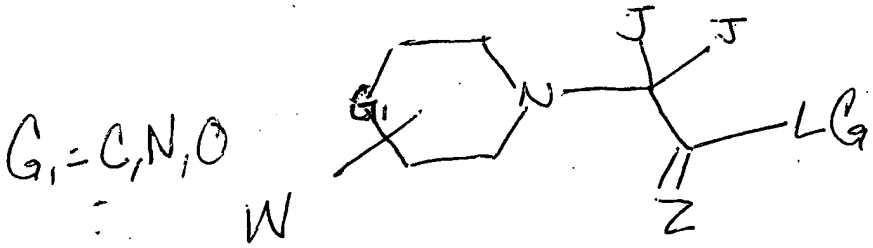
Earliest Priority Date: 1/27/04

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only ***Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.***

Please Search: the compound of Claim 71.



$G_1 = C, N, O$

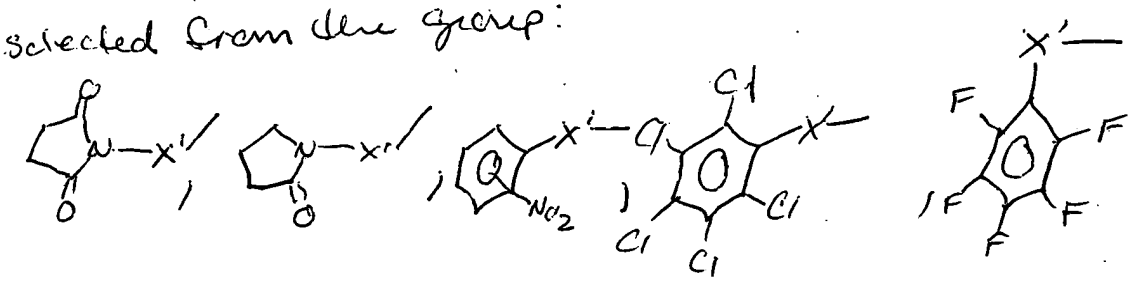
W

W = NH, NR^1, NR^2, PR^1, PR^2, O or S

J = H, deuterium(D), R^1, OR^1, SR^1, NHR^1, $N(R^1)_2$, Fluorine, Cl, Br, I

Z = O, S, NH, NR^1

LG = selected from the group:



X' = O or S

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=> d his ful

     (FILE 'HOME' ENTERED AT 10:18:35 ON 10 MAR 2006)

     FILE 'REGISTRY' ENTERED AT 10:18:44 ON 10 MAR 2006
L1             STR
L5          82 SEA SSS FUL L1
L6             STR
L7          46 SEA SUB=L5 SSS FUL L6

     FILE 'HCAPLUS' ENTERED AT 10:24:11 ON 10 MAR 2006
L8          29 SEA ABB=ON  PLU=ON  L7
               D STAT QUE L8
               D IBIB ABS HITSTR L8 1-29

     FILE 'REGISTRY' ENTERED AT 10:27:29 ON 10 MAR 2006
L9          36 SEA ABB=ON  PLU=ON  L5 NOT L7

     FILE 'HCAPLUS' ENTERED AT 10:27:38 ON 10 MAR 2006
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L11         17 SEA ABB=ON  PLU=ON  L10 NOT L8
               D STAT QUE
               D IBIB ABS HITSTR L11 1-17
L12        103 SEA ABB=ON  PLU=ON  ("PAPPIN D"/AU OR "PAPPIN D J"/AU OR
               "PAPPIN D J C"/AU OR "PAPPIN DARRYL"/AU OR "PAPPIN DARRYL
               J"/AU OR "PAPPIN DARRYL J C"/AU OR "PAPPIN DARRYL JOHN
               CECIL"/AU OR "PAPPIN DARYL"/AU) NOT (L8 OR L11)
L13          9 SEA ABB=ON  PLU=ON  ("BARTLET JONES M"/AU OR "BARTLET JONES
               MICHAEL"/AU) NOT (L8 OR L11)
               D STAT QUE L13
               D IBIB ABS L13 1-9
L14         97 SEA ABB=ON  PLU=ON  L12 NOT L13
L15         92 SEA ABB=ON  PLU=ON  L14 AND PD=<JANUARY 28, 2004
L16         38 SEA ABB=ON  PLU=ON  L15 AND ANALY?
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L18          6 SEA ABB=ON  PLU=ON  L17 NOT L7
               D STAT QUE
               D CN BRN MF FW STR RX 1-6


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
     provided by InfoChem.

     STRUCTURE FILE UPDATES:     8 MAR 2006  HIGHEST RN 876273-86-8
     DICTIONARY FILE UPDATES:    8 MAR 2006  HIGHEST RN 876273-86-8

     New CAS Information Use Policies, enter HELP USAGETERMS for details.

     TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

       Please note that search-term pricing does apply when
       conducting SmartSELECT searches.
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* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

FILE HCAPLUS

FILE COVERS 1907 - 10 Mar 2006 VOL 144 ISS 12
FILE LAST UPDATED: 9 Mar 2006 (20060309/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON JANUARY 17, 2006

FILE COVERS 1771 TO 2005.
FILE CONTAINS 9,428,406 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.                *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE   *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE          *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        *
* FOR PRICE INFORMATION SEE HELP COST                                *
**********************************************************************
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NEW

*** PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.**

*** NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.**

=>

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=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 10:24:11 ON 10 MAR 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 10 Mar 2006  VOL 144 ISS 12
FILE LAST UPDATED: 9 Mar 2006  (20060309/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=>
=>

=> d stat que l8
L1                STR
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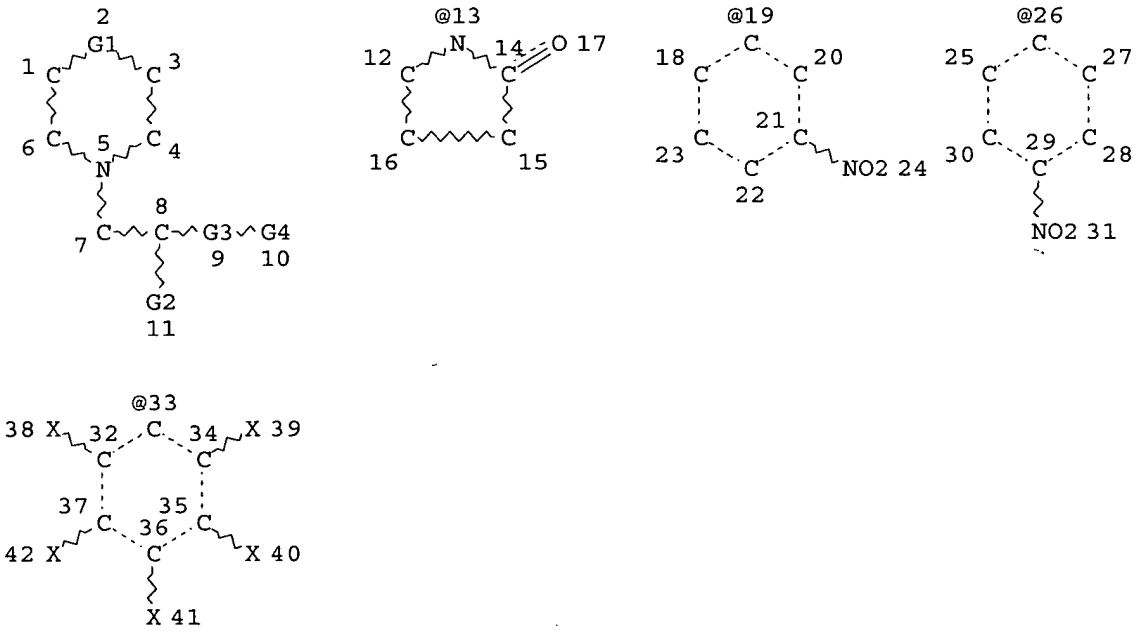


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VAR G3=O/S
VAR G4=13/19/26/33
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DEFAULT MLEVEL IS ATOM
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
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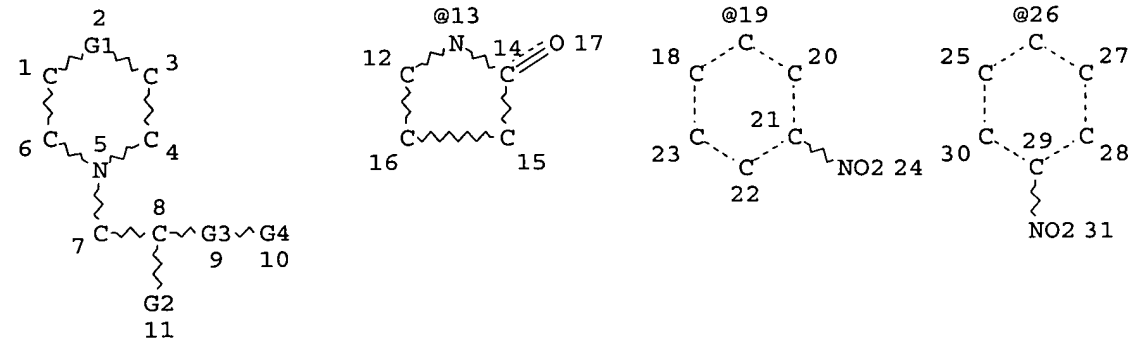
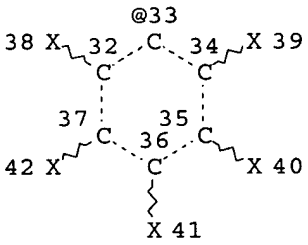
L6 STR





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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L7 46 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L8 29 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

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=> d ibib abs hitstr l8 1-29

L8 ANSWER 1 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:592130 HCAPLUS
DOCUMENT NUMBER: 143:115574
TITLE: Preparation of isotopically enriched N-substituted piperazines
INVENTOR(S): Pappin, Darryl J. C.; Pillai, Sasi; Coull, James M.
PATENT ASSIGNEE(S): Applera Corp., USA

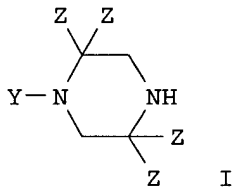
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148773	A1	20050707	US 2004-751388	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 2004-751353 A 20040105
US 2004-751354 A 20040105
US 2004-751387 A 20040105
US 2004-751388 A 20040105
US 2004-822639 A 20040412
US 2004-852730 A 20040524

OTHER SOURCE(S): MARPAT 143:115574
GI



I

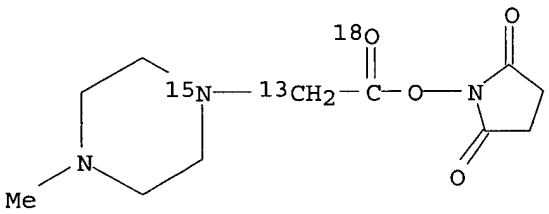
AB Isotopically enriched N-substituted piperazines (I) or salts thereof, comprising one or more heavy atom isotopes (Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or fluorine atoms; Z = independently H, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H or F atoms, a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms), or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group; wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked hydrogen or fluorine atoms; wherein the N-methylpiperazine is isotopically enriched with either of 13C and/or 15N) are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids

which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like (no data). Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)

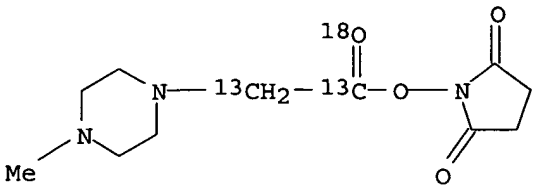


●2 HCl

IT **856188-16-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856188-16-4 HCAPLUS

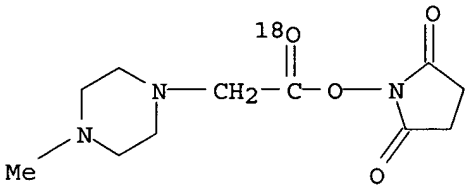
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **856187-87-6P 856188-06-2P 857027-09-9P**
857027-10-2P 857503-00-5P 857503-01-6P
857503-03-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazines as isobaric labeling reagents)

RN 856187-87-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



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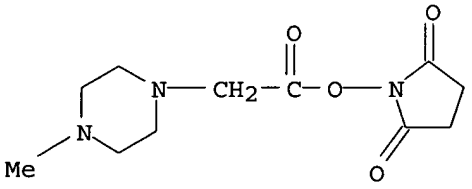

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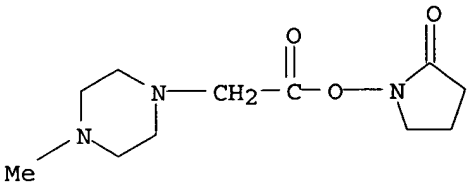

RN 857027-10-2 HCAPLUS
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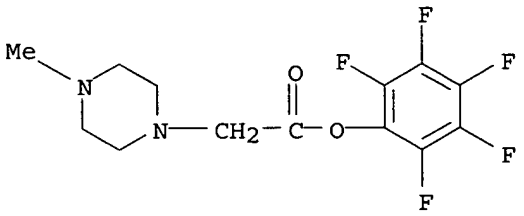

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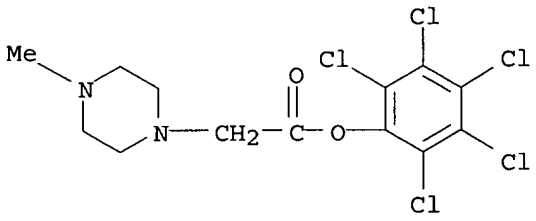

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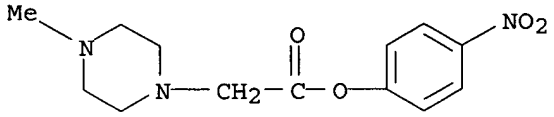

RN 857503-03-8 HCAPLUS
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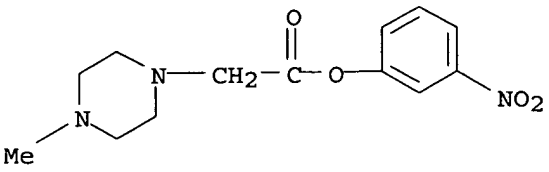

L8 ANSWER 2 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:592129 HCAPLUS
DOCUMENT NUMBER: 143:97398
TITLE: Preparation of active esters of N-substituted piperazine acetic acids, including isotopically enriched versions
INVENTOR(S): Dey, Subhakar; Pappin, Darryl J. C.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 33 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148771	A1	20050707	US 2004-751354	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:97398
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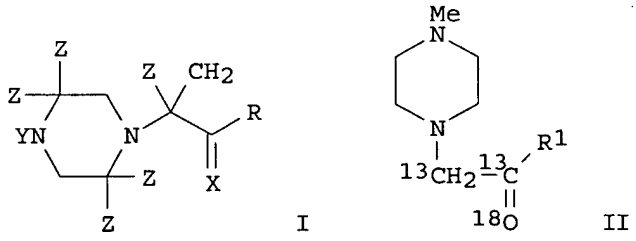


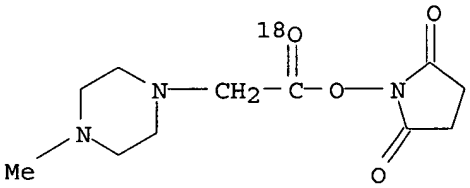
I

II

AB In some embodiments, this invention pertains to active esters of N-substituted piperazine acetic acid I (R = leaving group; X = O, S; Y = C1-C6 alkyl, C1-C6 alkyl ether; Z = H, 2H, F, Cl, Br, iodide, amino acid side chain, C1-C6 alkyl, C1-C6 alkyl ether), including isotopically enriched versions thereof. In some embodiments, this invention pertains to methods for the preparation of active esters of N-substituted piperazine acetic acid, including isotopically enriched versions thereof. For example, the isotopically labeled N-methylpiperazine II (R1 = 18OH) reacted with the trifluoroacetic acid ester of N-hydroxysuccinimide to give the succinate II (R1 = OR2, R2 = succinimido).

IT **856187-87-6P 856188-06-2P 856188-16-4P 856188-20-0P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of active esters of N-substituted piperazine acetic acids and their labeled derivs.)

RN 856187-87-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



RN 856188-06-2 HCAPLUS
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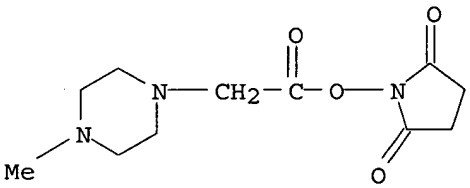
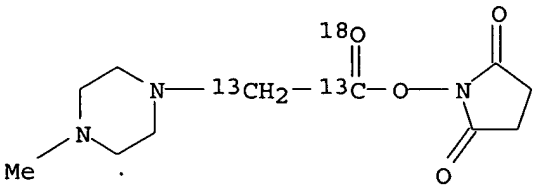
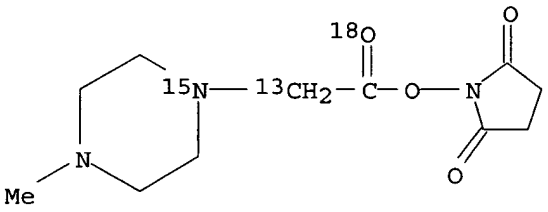


RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L8 ANSWER 3 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:592027 HCAPLUS
DOCUMENT NUMBER: 143:93642
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 36 pp., Cont.-in-part of U.S. Ser. No. 751,353.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A2	20040412
US 2004-852730	A	20040524

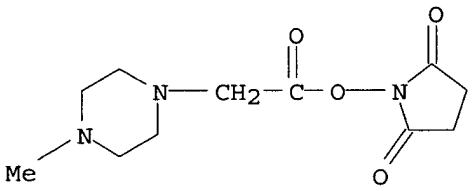
OTHER SOURCE(S): MARPAT 143:93642

AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.

IT **856188-06-2P 857027-09-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

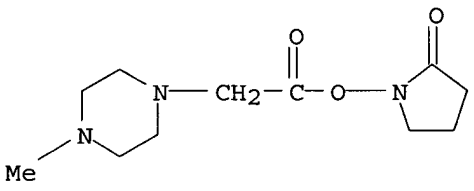
RN 856188-06-2 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



RN 857027-09-9 HCAPLUS

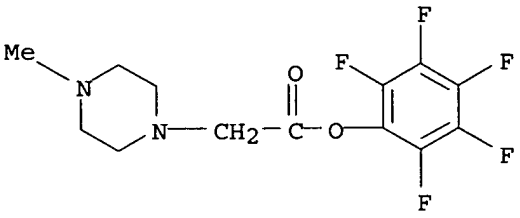
CN 2-Pyrrolidinone, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



IT **856187-87-6P 856188-16-4P 856188-20-0P 857027-10-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)

RN 856187-87-6 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:588426 HCAPLUS
DOCUMENT NUMBER: 143:115568
TITLE: Preparation of isotopically enriched N-substituted piperazine-1-acetic acids
INVENTOR(S): Dey, Subhakar; Pappin, Darryl J. c.; Purkayastha, Subhasish; Pillai, Sasi; Coull, James M.
PATENT ASSIGNEE(S): Applera Corp., USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

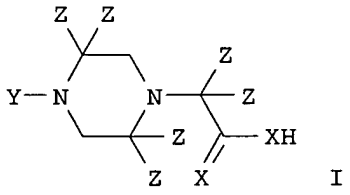
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148774	A1	20050707	US 2004-751387	20040105
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2004-751353	A	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A	20040412
US 2004-852730	A	20040524

OTHER SOURCE(S): MARPAT 143:115568
GI



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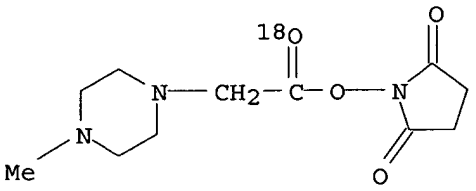
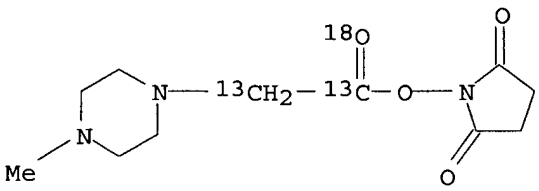
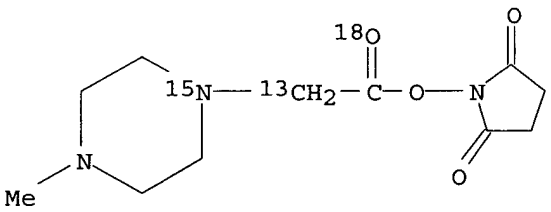


RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 856188-20-0 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

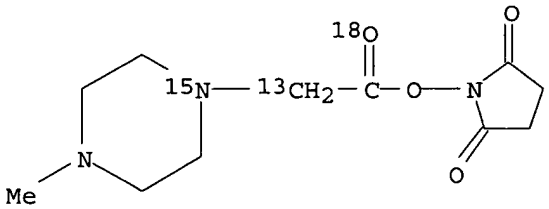
RN 857027-10-2 HCAPLUS
CN 1-Piperazineacetic acid, 4-methyl-, pentafluorophenyl ester (9CI) (CA INDEX NAME)

AB Isotopically enriched N-substituted piperazine-1-acetic acids (I) or salts thereof, comprising one or more heavy atom isotopes [X = O, S; Y = straight chain or branched C1-6 alkyl or C1-6 alkyl ether group wherein the carbon atoms of the alkyl group or alkyl ether group each independently comprise linked hydrogen, deuterium or F atoms; Z = independently H, deuterium, F, Cl, Br, iodine, an amino acid side chain, a straight chain or branched C1-6 alkyl group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms), a straight chain or branched C1-6 alkyl ether group that may optionally contain a substituted or unsubstituted aryl group wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms, or a straight chain or branched C1-6 alkoxy group that may optionally contain a substituted or unsubstituted aryl group (wherein the carbon atoms of the alkyl and aryl groups each independently comprise linked H, deuterium or F atoms)] are prepared N-substituted piperazines can be used as intermediates in the synthesis of N-substituted piperazine acetic acids which in turn can be used as intermediates in the synthesis of active esters of N-substituted piperazine acetic acid. The active esters of N-substituted piperazine acetic acid can be used as labeling reagents to prepare a set of isobaric labeling reagents. The set of isobaric labeling reagents can be used to label analytes such as peptides, proteins, amino acids, oligonucleotides, DNA, RNA, lipids, carbohydrates, steroids, small mols. and the like. Thus, to a stirring solution of 1.18 g (11.83 mmol) N-methylpiperazine in 15 mL toluene at room temperature was added 1 g (5.91 mmol) of Et bromoacetate-1,2-13C dropwise, over a period of 15 min. The reaction mixture was then heated in an oil bath at 90° for 4 h, cooled to room temperature, filtered to remove the off-white solid to give, after workup on the combined filtrate and washings, 1.10 g (quant.) of 4-methylpiperazine-1-acetic acid Et ester-1,2-13C (II) as an off-white oil. II (1.1 g) was refluxed in water for 24 h to give 780 mg 4-methylpiperazine-1-acetic acid-1,2-13C.

IT **856188-20-0P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)

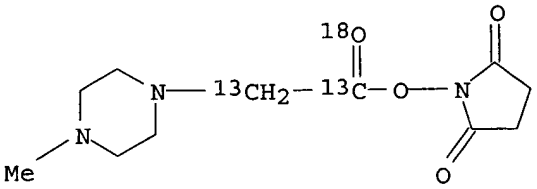
RN 856188-20-0 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl-1-15N)acetyl-2-13C-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



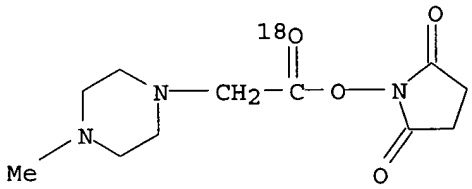
●2 HCl

IT **856188-16-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
RN 856188-16-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-13C2-18O]oxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **856187-87-6P 856188-06-2P 857027-09-9P**
857027-10-2P 857503-00-5P 857503-01-6P
857503-03-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of isotopically enriched N-substituted piperazine-1-acetic acids as isobaric labeling reagents)
RN 856187-87-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



RN 856188-06-2 HCAPLUS
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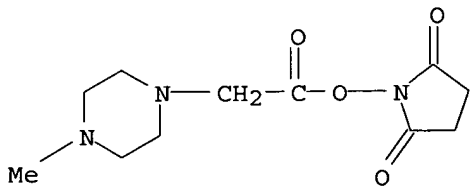
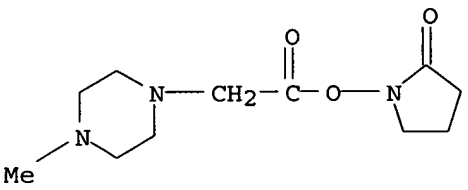
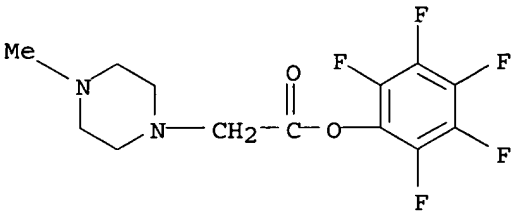


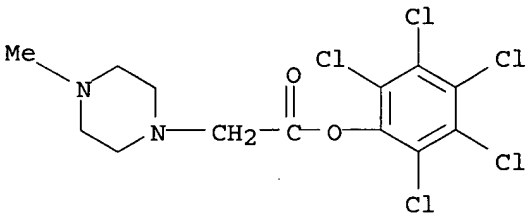
RN 857027-09-9 HCAPLUS
CN 2-Pyrrolidinone, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



RN 857027-10-2 HCAPLUS
CN 1-Piperazineacetic acid, 4-methyl-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



RN 857503-00-5 HCAPLUS
CN 1-Piperazineacetic acid, 4-methyl-, pentachlorophenyl ester (9CI) (CA INDEX NAME)



RN 857503-01-6 HCAPLUS
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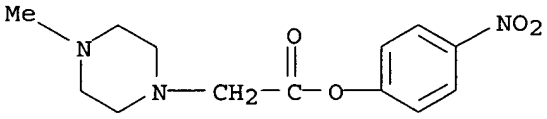

RN 857503-03-8 HCAPLUS
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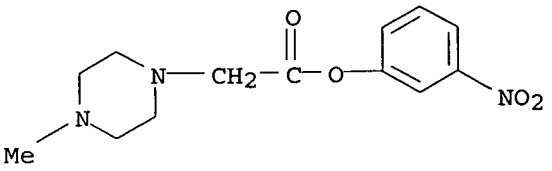


L8 ANSWER 5 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:588349 HCAPLUS
DOCUMENT NUMBER: 143:112150
TITLE: Isobarically labeled analytes and fragment ions derived therefrom
INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 88 pp., Cont.-in-part of U.S. Ser. No. 822,639.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

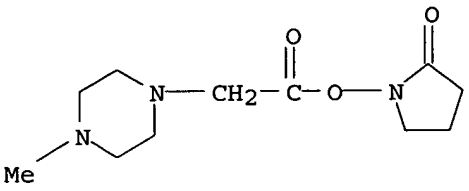
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005148087	A1	20050707	US 2004-852730	20040524
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

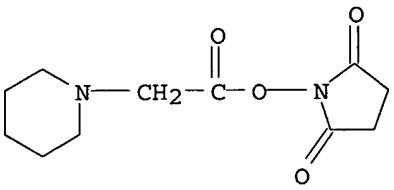
PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-822639	A2	20040412
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-852730	A	20040524

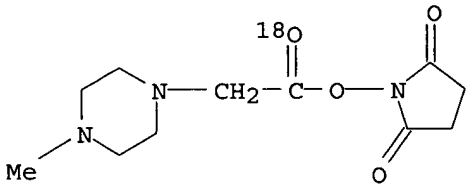
OTHER SOURCE(S): MARPAT 143:112150
AB This invention pertains to isobarically labeled analytes and fragment ions thereof.
IT **857027-09-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isobarically labeled analytes and fragment ions derived therefrom)
RN 857027-09-9 HCAPLUS
CN 2-Pyrrolidinone, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



IT **741683-79-4P 856187-87-6P 856188-06-2P**
857027-10-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(isobarically labeled analytes and fragment ions derived therefrom)
RN 741683-79-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl)oxy]- (9CI) (CA INDEX NAME)



RN 856187-87-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



RN 856188-06-2 HCAPLUS
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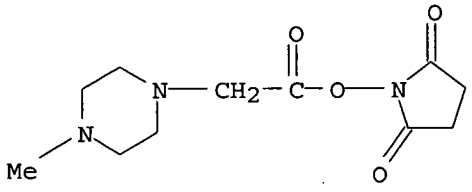
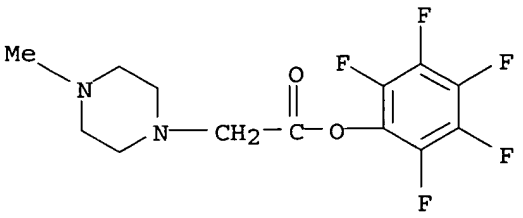


RN 857027-10-2 HCAPLUS
CN 1-Piperazineacetic acid, 4-methyl-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:588336 HCAPLUS
DOCUMENT NUMBER: 143:93635
TITLE: Mixtures of isobarically labeled analytes and fragments ions derived therefrom
INVENTOR(S): Pappin, Darryl J. C.; Purkayastha, Subhasish; Coull, James M.
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 29 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

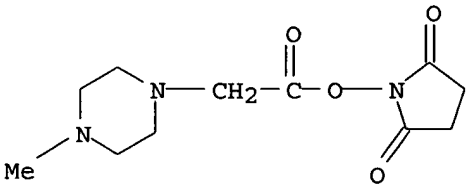
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005147982	A1	20050707	US 2004-751353	20040105
US 2005147985	A1	20050707	US 2004-822639	20040412
US 2005148087	A1	20050707	US 2004-852730	20040524
WO 2005068446	A1	20050728	WO 2005-US223	20050105

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

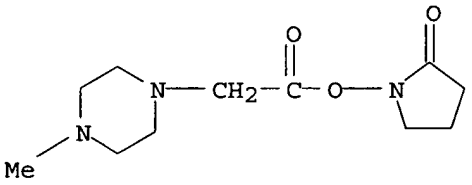
PRIORITY APPLN. INFO.:

US 2004-751353	A2	20040105
US 2004-751354	A	20040105
US 2004-751387	A	20040105
US 2004-751388	A	20040105
US 2004-822639	A2	20040412
US 2004-852730	A	20040524

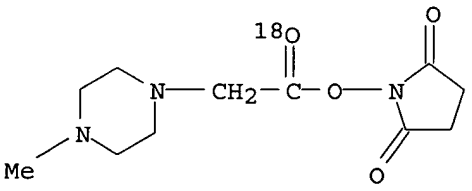
AB This invention pertains to mixts. of isobarically labeled analytes and fragment ions thereof.
IT **856188-06-2P 857027-09-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856188-06-2 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



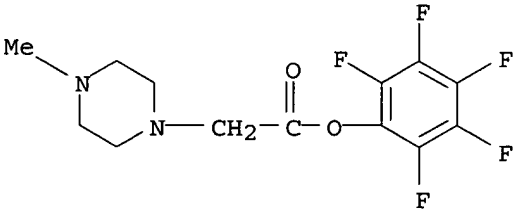
RN 857027-09-9 HCAPLUS
CN 2-Pyrrolidinone, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



IT **856187-87-6P 857027-10-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(mixts. of isobarically labeled analytes and fragments ions derived therefrom)
RN 856187-87-6 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl-18O]oxy]- (9CI) (CA INDEX NAME)



RN 857027-10-2 HCAPLUS
CN 1-Piperazineacetic acid, 4-methyl-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



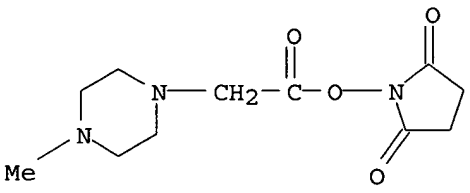
L8 ANSWER 7 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:412987 HCAPLUS

DOCUMENT NUMBER: 144:186804
TITLE: Analysis of cell membrane aminophospholipids as isotope-tagged derivatives
AUTHOR(S): Zemski Berry, Karin A.; Murphy, Robert C.
CORPORATE SOURCE: Department of Pharmacology, University of Colorado Health Sciences Center, Aurora, CO, 80045, USA
SOURCE: Journal of Lipid Research (2005), 46(5), 1038-1046
CODEN: JLPRAW; ISSN: 0022-2275
PUBLISHER: American Society for Biochemistry and Molecular Biology, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Glycerophosphoethanolamine (GPEtn) and glycerophosphoserine (GPSer) lipids were reacted with a multiplexed set of differentially isotopically enriched N-methylpiperazine acetic acid N-hydroxysuccinimide ester reagents, which place isobaric mass labels at a primary amino group. The resulting derivitized aminophospholipids were isobaric and chromatog. indistinguishable but yielded pos. reporter ions (m/z 114 or 117) after collisional activation that could be used to identify and quantify individual members of the multiplex set. The chromatog. and mass spectrometric response of N-methylpiperazine amide-tagged aminophospholipids was probed using glycerophosphoethanolamine and glycerophosphoserine lipid stds. The [M+H]+ of each tagged aminophospholipid shifted 144 Da, and during collision-induced dissociation the major fragmentation ion was either m/z 114 or 117. This mode of detecting aminophospholipids was useful for an unbiased anal. of plasmalogen GPEtn lipids. Mol. species information on the esterified fatty acyl substituents was obtained by collisional activation of the [M-H]- ions. The isotope-tagged reagents were used to assess changes in the distribution of GPEtn lipids after exposure of liposomes made from phospholipids extracted from RAW 264.7 cells to Cu2+/H2O2 to illustrate the ability of these reagents to aid in the mass spectrometric identification of aminophospholipid changes that occur during biol. stimuli.

IT **856188-06-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and mass spectrometric anal. of cell membrane aminophospholipids as isotope-tagged derivs.)

RN 856188-06-2 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(4-methyl-1-piperazinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:271531 HCAPLUS
DOCUMENT NUMBER: 142:492702
TITLE: Coordination Behavior toward Copper(II) and Zinc(II) Ions of Three Ligands Joining 3-Hydroxy-2-pyridinone and Polyaza Fragments

AUTHOR(S): Ambrosi, Gianluca; Formica, Mauro; Fusi, Vieri; Giorgi, Luca; Guerri, Annalisa; Lucarini, Simone; Micheloni, Mauro; Paoli, Paola; Rossi, Patrizia; Zappia, Giovanni
CORPORATE SOURCE: Institute of Chemical Sciences and Institute of Pharmaceutical Chemistry, University of Urbino, Urbino, I-61029, Italy
SOURCE: Inorganic Chemistry (2005), 44(9), 3249-3260
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

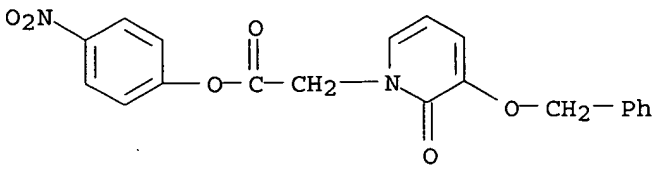
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis and characterization of new polydentate ligand 2-(N),2'-(N')-bis[2-(3-hydroxy-2-oxo-2H-pyridin-1-yl)acetamido]-1(N'),2(N),2'(N')-trimethyl-2,2'-diaminodiethylamine, I (L3), is reported. The coordination properties of L3 and of two analogous macrocyclic ligands II [Z = H2, (L1) and Z = O (L2)] toward Cu(II) and Zn(II) metal ions are reported. All three ligands show the 3-hydroxy-2(1H)-pyridinone (HPO) groups attached as sidearms to a polyaza fragment, which is a macrocyclic framework in the case of L1 and L2 while it is an open chain in the case of L3. The role of the polyaza fragments in preorganizing the two sidearms was studied. The basicity of L3 and the binding properties of L1-L3 were determined by potentiometric measurements in aqueous solution (298.1 ± 0.1 K, I = 0.15 mol dm-3). UV-visible spectra as well 1H and 13C NMR expts. were used to understand the role of the HPO and of the polyaza fragments in the stabilization of the cations. While L1 forms stable mono- and dinuclear complexes, L2 and L3 can form only mononuclear species with each of the metal ions studied. In the main mononuclear species of L2 and L3, the two HPO moieties stabilize the M(II) in a square-planar geometry due to the two O atoms of each HPO. The coordination sphere of the metal is completed by adding a secondary ligand such as H2O mols. in the case of Cu(II) systems or OH- in the Zn(II) systems. These results are confirmed by the crystal structures of the [CuH-1L2]+ and [CuH-1L3]+ species reported herein. Two conformations of L1 can be hypothesized in the formation of the dinuclear species, as suggested by NMR expts. on the [ZnH-2L1] species, which shows two conformers slowly interchanging on the NMR time scale, one of which is more insol.

IT **852159-56-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of polyaza hydroxypyridinone-containing ligand)

RN 852159-56-9 HCAPLUS

CN 1(2H)-Pyridineacetic acid, 2-oxo-3-(phenylmethoxy)-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:824132 HCAPLUS
DOCUMENT NUMBER: 141:310231
TITLE: Mass labels
INVENTOR(S): Hamon, Christian; Kuhn, Karsten; Thompson, Andrew; Reuschling, Dieter; Schaefer, Juergen
PATENT ASSIGNEE(S): Xzillion G.m.b.H. & Co. K.-G., Germany; Proteome Sciences PLC
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

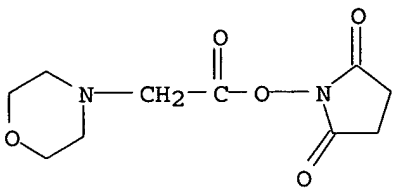
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004086050	A2	20041007	WO 2004-GB1167	20040318
WO 2004086050	A3	20041229		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2520297	AA	20041007	CA 2004-2520297	20040318
EP 1606623	A2	20051221	EP 2004-721565	20040318
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
NO 2005004684	A	20051012	NO 2005-4684	20051012
PRIORITY APPLN. INFO.:			GB 2003-6756 A	20030324
			WO 2004-GB1167 W	20040318

AB Provided is a method for characterizing a mol. by mass spectrometry, which mol. comprises one or more free amino groups, which method comprises: (a) reacting one or more free amino groups in the mol. with a mass tag reagent comprising a reactive functionality capable of reacting with an amino group, and a tertiary amino group linked to the reactive functionality; and (b) characterizing the mol. by mass spectrometry.

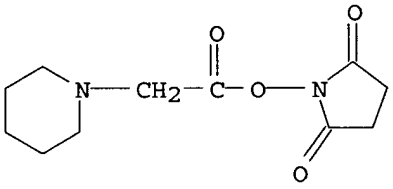
IT **741683-76-1P 741683-79-4P 768385-34-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mass labels)

RN 741683-76-1 HCAPLUS

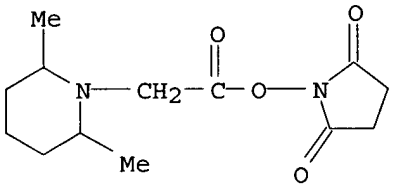
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME)



RN 741683-79-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl)oxy]- (9CI) (CA INDEX NAME)



RN 768385-34-8 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(2,6-dimethyl-1-piperidinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 10 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:681717 HCAPLUS
DOCUMENT NUMBER: 141:202794
TITLE: Methods, mixtures, kits and compositions pertaining to analyte determination
INVENTOR(S): Pappin, Darryl J. C.; Bartlet-Jones, Michael
PATENT ASSIGNEE(S): Applera Corporation, USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004070352	A2	20040819	WO 2004-US2077	20040127

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2488584	AA	20040819	CA 2004-2488584	20040127
US 2004219685	A1	20041104	US 2004-765264	20040127
US 2004220412	A1	20041104	US 2004-765267	20040127
US 2004219686	A1	20041104	US 2004-765458	20040127
EP 1588145	A2	20051026	EP 2004-705571	20040127

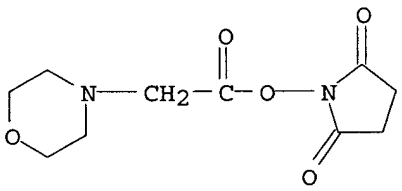
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

PRIORITY APPLN. INFO.: US 2003-443612P P 20030130
WO 2004-US2077 W 20040127

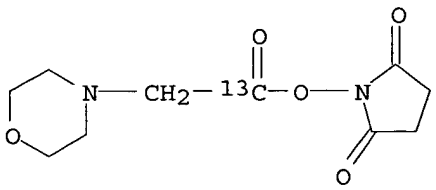
AB This invention pertains to methods, mixts., kits and/or compns. for the determination of analytes by mass anal. using unique labeling reagents or sets of unique labeling reagents. The labeling reagents can be isomeric or isobaric and can be used to produce mixts. suitable for multiplex anal. of the labeled analytes.

IT **741683-76-1P 741683-77-2P 741683-78-3P 741683-79-4P 741683-80-7P 741683-86-3P 741683-93-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(methods, mixts., kits and compns. pertaining to analyte determination)

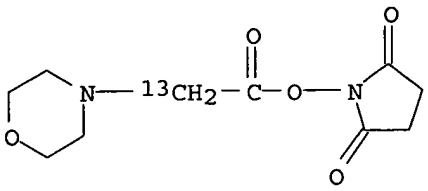
RN 741683-76-1 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl)oxy]- (9CI) (CA INDEX NAME)



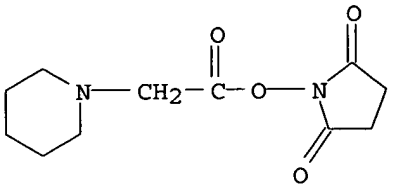
RN 741683-77-2 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)



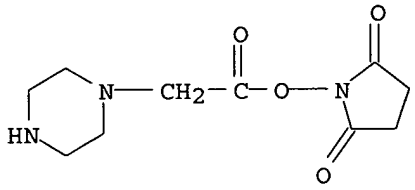
RN 741683-78-3 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(4-morpholinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)



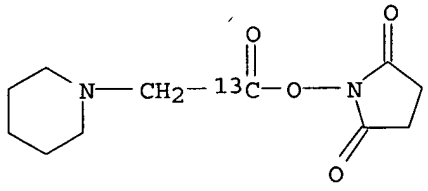
RN 741683-79-4 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl)oxy]- (9CI) (CA INDEX NAME)



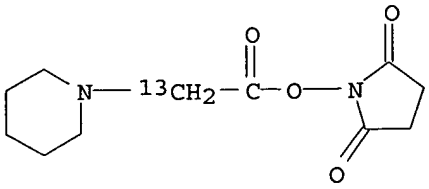
RN 741683-80-7 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperazinylacetyl)oxy]- (9CI) (CA INDEX NAME)



RN 741683-86-3 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-1-13C)oxy]- (9CI) (CA INDEX NAME)



RN 741683-93-2 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[(1-piperidinylacetyl-2-13C)oxy]- (9CI) (CA INDEX NAME)



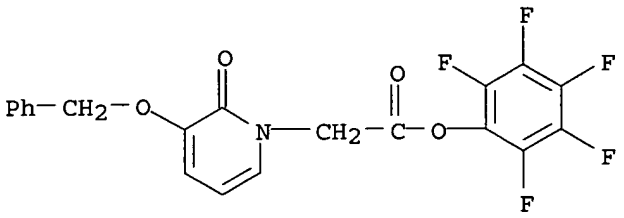
L8 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:984421 HCAPLUS
DOCUMENT NUMBER: 140:163851
TITLE: New ligand bearing preorganized binding side-arms interacting with ammonium cations: synthesis, conformational studies and crystal structure
AUTHOR(S): Formica, Mauro; Fusi, Vieri; Giorgi, Luca; Guerri, Annalisa; Sucarini, Simone; Micheloni, Mauro; Paoli, Paola; Pontellini, Roberto; Rossi, Patrizia; Tarzia, Giorgio; Zappia, Giovanni
CORPORATE SOURCE: Institute of Chemical Sciences, University of Urbino, Urbino, I-61029, Italy
SOURCE: New Journal of Chemistry (2003), 27(11), 1575-1583
CODEN: NJCHE5; ISSN: 1144-0546
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:163851

AB The synthesis and characterization of the new tetraazamacrocycle 4-(N)-bis[2-(3-hydroxy-2-oxo-2H-pyridin-1-yl)acetamido]-1,7-dimethyl-1,4,7,10-tetraazacyclododecane (I) is reported. I shows two 3-(hydroxy)-1-(carbonylmethylen)-2-(1H)-pyridinone moieties as side-arms of a tetra-aza-macrocyclic base. The key coupling of side-arms was studied and the most significant results were obtained by activating the 3-(benzyloxy)-1-(carboxymethyl)-2-(1H)-pyridinone as a pentafluorophenol ester. The acid-base properties of I and its capability to interact with simple ammonium cations were investigated by potentiometric measurements in aqueous solution (298.1±0.1 K, I = 0.15 mol dm-3). Protonated species of I can bind NH4+ or primary ammonium cations such as MeNH3+ which are not bound in aqueous solution 1H and 13C NMR spectra showed the existence in solution of two conformers on the NMR time scale due to the rotational restriction of the two N-C=O groups. The activation parameters were determined by dynamic variable-temperature NMR anal. Mol. dynamics calcns. gave results in agreement with the exptl. data for both conformation and ammonium-binding studies, underlining that the transformation of the two secondary amines of the macrocyclic base to amide functions, forces the side-arms to remain fixed in position, almost face to face and thus to be preorganized to interact with other species. The crystal structure of the [HL]Cl.8H2O species shows the high number of preorganized hydrogen bond sites capable, in this case, of interacting directly with five H2O mols.

IT **654637-03-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(coupling reaction of; preparation and potentiometric titration of multidentate azacrown ether ligand bearing preorganized binding side-arms interacting with ammonium cations)

RN 654637-03-3 HCAPLUS

CN 1(2H)-Pyridineacetic acid, 2-oxo-3-(phenylmethoxy)-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

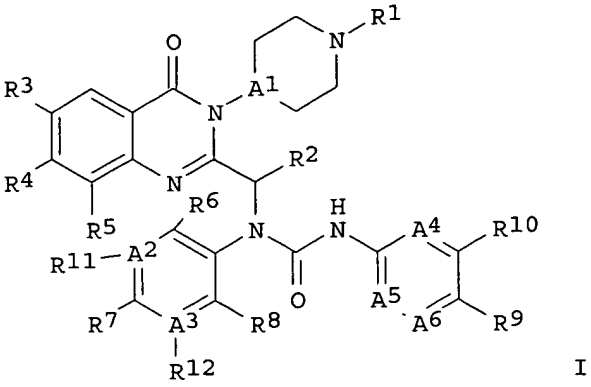
L8 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:930975 HCAPLUS
DOCUMENT NUMBER: 139:395945
TITLE: Preparation of quinazolinylmethyl urea derivatives as fungal efflux pump inhibitors
INVENTOR(S): Watkins, Will J.; Lemoine, Remy; Cho, Aesop; Palme, Monica
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 109 pp., Cont.-in-part of U.S. Ser. No. 906,864.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003220338	A1	20031127	US 2002-243074	20020912
US 6596723	B1	20030722	US 2001-906864	20010716
US 2003229097	A1	20031211	US 2002-334755	20021230
US 6689782	B2	20040210		
WO 2004024140	A1	20040325	WO 2003-US5184	20030221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003215343	A1	20040430	AU 2003-215343	20030221

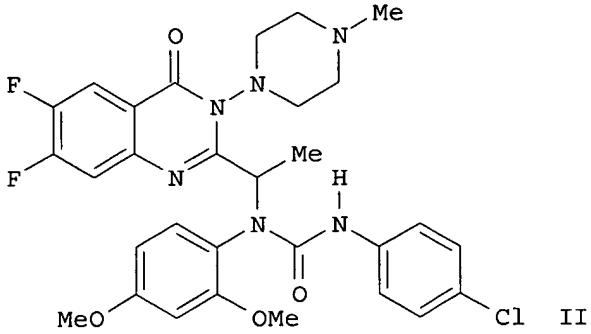
PRIORITY APPLN. INFO.:

US 2001-906864	A2	20010716
US 2002-243074	A2	20020912
US 2002-334755	A	20021230
WO 2003-US5184	W	20030221

OTHER SOURCE(S): MARPAT 139:395945
GI



I



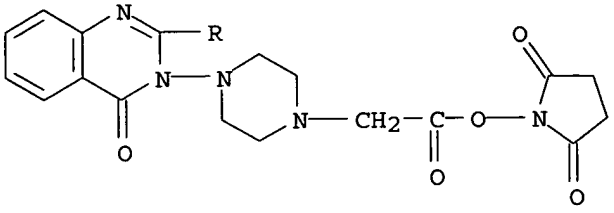
II

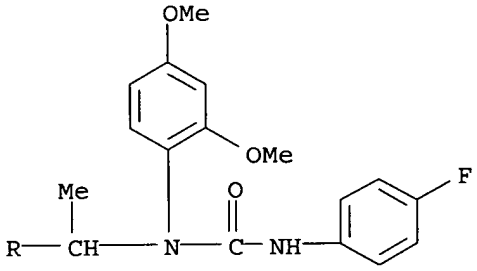
AB This invention relates to compds. of formula I [A1-A6 = C, N; R1 = H, alkyl, cycloalkyl, CH2-cycloalkyl, etc.; R2 = alkyl; R3-R12 = H, alkyl, CF3, alkoxy, halo, OH, CN, etc.] that are efflux pump inhibitors and therefore are useful as potentiators of anti-fungal agents for the treatment of infections caused by fungi that employ an efflux pump resistance mechanism. Thus, II was prepared and showed a reduced MIC value against Candida albicans in the presence of fluconazole.

IT **626245-59-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinazolinylmethyl urea derivs. as fungal efflux pump inhibitors)

RN 626245-59-8 HCAPLUS

CN Urea, N-(2,4-dimethoxyphenyl)-N-[1-[3-[4-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-1-piperazinyl]-3,4-dihydro-4-oxo-2-quinazolinyl]ethyl]-N'-(4-fluorophenyl)- (9CI) (CA INDEX NAME)





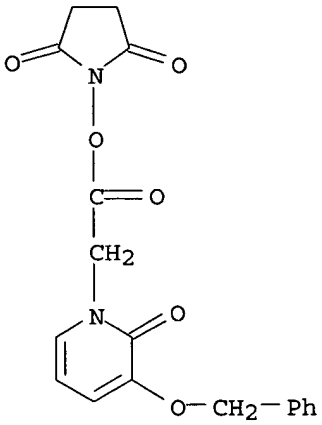
L8 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:439195 HCAPLUS
DOCUMENT NUMBER: 131:184754
TITLE: Synthesis of 3-Hydroxy-2-pyridinone Derivatives of 4-tert-Butylcalix[4]arenes: A New Class of Selective Extractants of Actinide(IV) Ions
AUTHOR(S): Lambert, Timothy N.; Dasaradhi, Lakkaraju; Huber, Vincent J.; Gopalan, Aravamudan S.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM, 88003-8001, USA
SOURCE: Journal of Organic Chemistry (1999), 64(16), 6097-6101
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:184754
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Two hydroxypyridinone calixarene derivs. I (n = 3; X = NH; X1 = O; n = 2; X = O; X1 = H2) have been developed as a new class of extractants for actinides. I proved efficient for extracting Th(IV) and Fe(III) and selective for Th(IV) under competitive conditions.

IT **95215-73-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of hydroxypyridinone derivs. of calixarenes as selective extractants of actinide (IV) ions)

RN 95215-73-9 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)

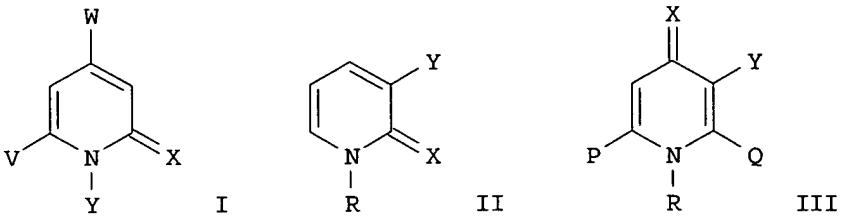


REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:402422 HCAPLUS
DOCUMENT NUMBER: 129:81670
TITLE: Preparation of therapeutic antioxidants for Alzheimer's disease
INVENTOR(S): Tilbrook, Gary Stuart; Hider, Robert Charles; Moridani, Majid Yousefi
PATENT ASSIGNEE(S): Cenes Ltd., UK; Tilbrook, Gary Stuart; Hider, Robert Charles; Moridani, Majid Yousefi
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9825905	A2	19980618	WO 1997-GB3306		19971210
WO 9825905	A3	19981029			
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9878471	A1	19980703	AU 1998-78471		19971210
PRIORITY APPLN. INFO.:			GB 1996-25638	A	19961210
			WO 1997-GB3306	W	19971210

OTHER SOURCE(S): MARPAT 129:81670
GI



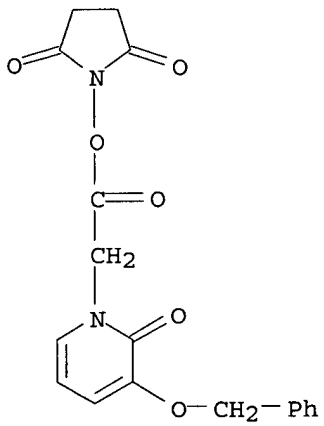
I II III

AB The title compds. [I (wherein X = S, O; Y = OR1, SR1; R1 = H, lower alkyl; W, V = OH, NO2, CF3, etc.), II (X = S, O; Y = OR1, SR1; R, R1 = H, lower alkyl, (CH2)nSH, etc.; n = 1-4), III (P, Q = H, lower alkyl, NH2CH2, etc.)], useful for therapy and prophylaxis of neurodegenerative disease such as Alzheimer's disease, were prepared Thus, treatment of 3-hydroxy-2(1H)-pyridinone with MeI in a sealed glass tube at 140° afforded 59% II [X = O; Y = OH; R = Me] which showed IC50 of 46 μM against tyrosine nitration and IC50 of 420 μM against lipid peroxidn.

IT **95215-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of therapeutic antioxidants for Alzheimer's disease)

RN 95215-73-9 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 15 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:319625 HCAPLUS

DOCUMENT NUMBER: 129:54280

TITLE: Synthetic studies into 3-hydroxy-2(1)-pyridinone based hexadentate metal(III) ion chelators

AUTHOR(S): Fox, Raymond C.; Taylor, Paul D.

CORPORATE SOURCE: Chemistry and Life Sciences, Research Triangle Institute, Research Triangle Park, NC, 27709, USA

SOURCE: Synthetic Communications (1998), 28(9), 1563-1574
CODEN: SYNCAV; ISSN: 0039-7911

PUBLISHER: Marcel Dekker, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

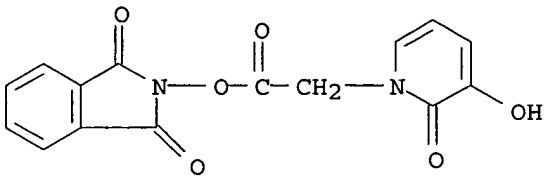
OTHER SOURCE(S): CASREACT 129:54280

AB An improved synthesis and purification of the hexadentate chelators, N,N,N,-tris[2-(3-hydroxy-2-oxo-1,2-dihydropyridin-1-yl)acetamido]ethylamine and N,N,N,-tris[2-(3-hydroxy-4-methyl-2-oxo-1,2-dihydropyridin-1-yl)acetamido]ethylamine is described.

IT **208592-19-2P 208592-20-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of hydroxypyridinone-based hexadentate metal ion chelators)

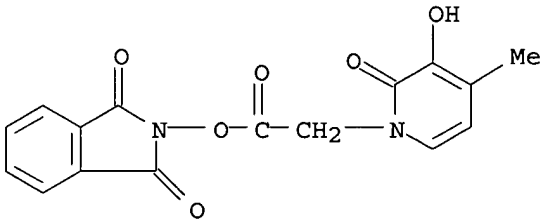
RN 208592-19-2 HCAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[(3-hydroxy-2-oxo-1(2H)-pyridinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



RN 208592-20-5 HCAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[(3-hydroxy-4-methyl-2-oxo-1(2H)-pyridinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 16 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:805833 HCAPLUS

DOCUMENT NUMBER: 128:58278

TITLE: Nucleic acid hybridization using probes labeled with a reporter group with spectroscopic properties sensitive to hybrid formation

INVENTOR(S): Kubista, Mikael; Svanvik, Nicke

PATENT ASSIGNEE(S): Kubista, Mikael, Swed.; Svanvik, Nicke

SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9745539	A1	19971204	WO 1997-SE953	19970530

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ,

LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL,
PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ,
VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,
GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN,
ML, MR, NE, SN, TD, TG

SE 9602183	A	19971201	SE 1996-2183	19960531
SE 506700	C2	19980202		
CA 2256545	AA	19971204	CA 1997-2256545	19970530
CA 2451442	AA	19971204	CA 1997-2451442	19970530
AU 9731129	A1	19980105	AU 1997-31129	19970530
EP 918852	A1	19990602	EP 1997-926344	19970530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
BR 9709495	A	19990810	BR 1997-9495	19970530
CN 1226928	A	19990825	CN 1997-196872	19970530
JP 2000511057	T2	20000829	JP 1997-542246	19970530
EP 1357185	A1	20031029	EP 2003-11589	19970530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI				
RU 2223966	C2	20040220	RU 1998-123553	19970530
PL 188875	B1	20050531	PL 1997-366875	19970530
US 6329144	B1	20011211	US 1999-194679	19990129
AU 768137	B2	20031204	AU 2001-55970	20010725
AU 2001055970	A5	20010927		
JP 2005047901	A2	20050224	JP 2004-204075	20040712

PRIORITY APPLN. INFO.:	SE 1996-2183	A	19960531
	AU 1997-31129	A3	19970530
	CA 1997-2256545	A3	19970530
	JP 1997-542246	A3	19970530
	WO 1997-SE953	W	19970530
	EP 1997-926344	A3	19971204

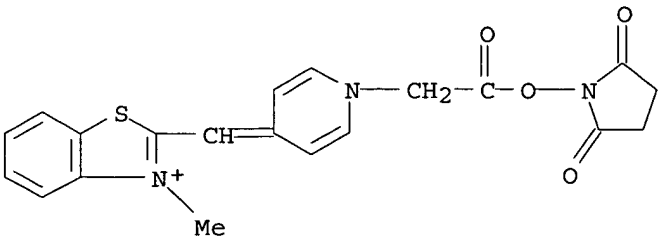
OTHER SOURCE(S): MARPAT 128:58278

AB Nucleic acid hybridization using probes labeled with a reporter group that changes its spectroscopic properties upon formation of a hybrid is described. The preferred reporter is an asym. cyanine dye. Use of such a probe allows the immediate or real time quantification of hybrid formation. The method can be used with nucleic acid probes or analogs such as peptide nucleic acids. A pair of suitable benzothiazol quinoline dyes were synthesized by standard chem and analogs with spacer arms prepared for conjugation to nucleic acids. A conjugate of one of these dyes bound to an immobilized peptide nucleic acid probe showed a 45-fold increase in fluorescence upon formation of a hybrid. Fluorescence showed up to a 50-fold increase in quantum yield (range 8-50-fold) depending upon the probe used.

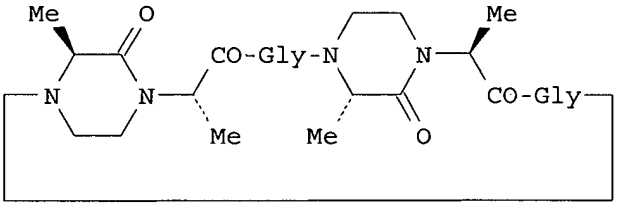
IT **200262-06-2P**
RL: ARU (Analytical role, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(as reporter group in nucleic acid hybridization; nucleic acid hybridization using probes labeled with reporter group with spectroscopic properties sensitive to hybrid formation)

RN 200262-06-2 HCAPLUS

CN Benzothiazolium, 2-[[1-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-4(1H)-pyridinylidene]methyl]-3-methyl- (9CI) (CA INDEX NAME)



L8 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:427460 HCAPLUS
DOCUMENT NUMBER: 123:83982
TITLE: Structure of cyclic hexa-pseudopeptide constructed from N,N'-ethylene-bridged-(S)-alanyl-(S)-alanine and glycine
AUTHOR(S): Kojima, Yoshitane; Yamashita, Tetsushi; Miyake, Hiroyuki
CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan
SOURCE: Chemistry Letters (1995), (3), 201-2
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

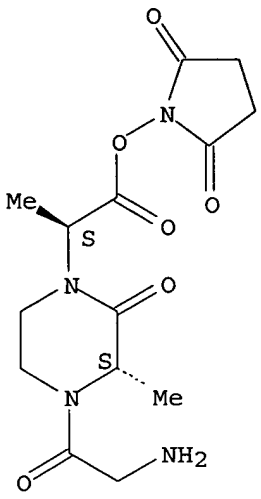
AB The crystal structure of 18-membered cyclic pseudopeptide I, containing N,N'-ethylene-bridged-(S)-alanyl-(S)-alanine and glycine was determined by x-ray crystallog. Moreover, the structure of this pseudopeptide was examined by 1H NMR measurement in CD3CN, and by mol. mechanics calcns.

IT **164857-03-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(structure of cyclic hexapseudopeptide constructed from ethylene-bridged alanylalanine and glycine)

RN 164857-03-8 HCAPLUS

CN Piperazinone, 4-(aminoacetyl)-1-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1-methyl-2-oxoethyl]-3-methyl-, monohydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L8 ANSWER 18 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:566123 HCAPLUS
DOCUMENT NUMBER: 117:166123
TITLE: Effect of the chemical modification by viologen on the reduction of metmyoglobin
AUTHOR(S): Tsukahara, Keiichi; Todorobaru, Hiromi
CORPORATE SOURCE: Fac. Sci., Nara Women's Univ., Nara, 630, Japan
SOURCE: Chemistry Letters (1992), (7), 1181-4
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English

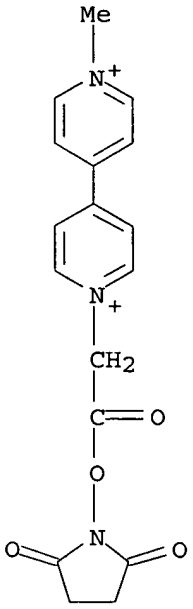
AB Metmyoglobin covalently linked with viologen was prepared and reduced by dithionite ions faster than the native metmyoglobin, suggesting that the reduction by dithionite of the attached viologen was followed by a rapid intramol. electron transfer from the viologen radical cation to the heme iron center.

IT **143674-76-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with metmyoglobin)

RN 143674-76-4 HCAPLUS
CN 4,4'-Bipyridinium, 1-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-1'-methyl-, diperchlorate (9CI) (CA INDEX NAME)

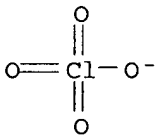
CM 1

CRN 143674-75-3
CMF C17 H17 N3 O4

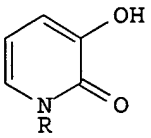


CM 2

CRN 14797-73-0
CMF Cl O4



L8 ANSWER 19 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:229683 HCAPLUS
DOCUMENT NUMBER: 112:229683
TITLE: Novel 3-hydroxy-2(1H)-pyridinones. Synthesis, iron(III)-chelating properties and biological activity
AUTHOR(S): Streater, Michael; Taylor, Paul D.; Hider, Robert C.; Porter, John
CORPORATE SOURCE: Dep. Chem. Biol. Chem., Univ. Essex, Colchester, CO4 3SQ, UK
SOURCE: Journal of Medicinal Chemistry (1990), 33(6), 1749-55
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:229683
GI



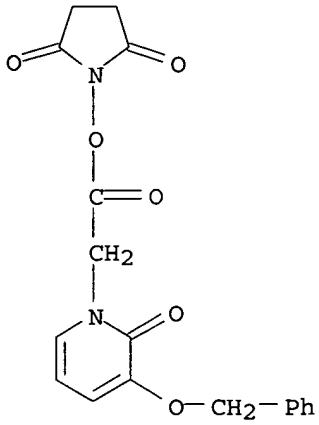
I

AB The synthesis of a range of novel bidentate, e.g., I (R = alkyl or alkylaminocarbonylmethyl), and hexadentate ligands containing the chelating moiety 3-hydroxy-2(1H)-pyridinone is described. The pKa values of the ligands and the stability consts. of their iron(III) complexes were determined The stability constant of the iron(III) complex of one of the hexadentate ligands is comparable to that of desferrioxamine B. The distribution coeffs. of the ligands and their iron(III) complexes were also determined One of the novel hexadentate compds. markedly enhanced iron(III) excretion from both hepatocytes and iron-overloaded mice.

IT **95215-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with amines)

RN 95215-73-9 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 20 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1990:7937 HCAPLUS

DOCUMENT NUMBER: 112:7937

TITLE: Preparation and testing of tripeptide derivatives as cardiovascular agents

INVENTOR(S): Sawayama, Tadahiro; Nishimura, Kazuya; Deguchi, Takashi

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

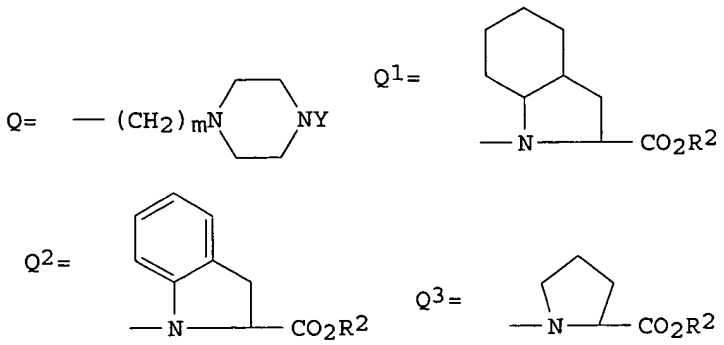
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 01125357	A2	19890517	JP 1987-281873	19871106
PRIORITY APPLN. INFO.:			JP 1987-281873	19871106
OTHER SOURCE(S):	MARPAT 112:7937			

GI



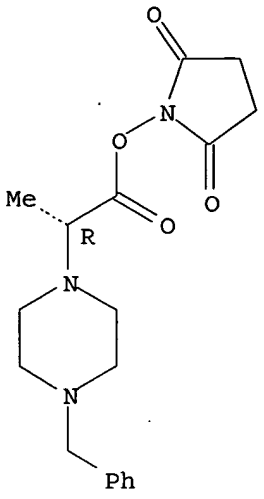
AB RR1CHCONHCH(CO2R2)(CH2)2COR3 [I; R = H, lower alkyl, PhCH2; R1 = (NH)m(CH2)nW, Q; R2 = H, lower alkyl; R3 = Q1, Q2, Q3, NR4CHR2CO2R2; W = H, CO2H, NH2, OH; Y = H, lower alkyl, Ph, PhCH2; R4 = C4-8 cycloalkyl, halo, alkoxy, (OH-substituted) Ph; m = 0, 1; n = 0-4] and their salts are prepared Refluxing 28 g 2-(S)-bromopropionic acid with 42 g PhCH2OH in PhMe gave 17.0 g benzyl 2-(S)-bromopropionate, 2.2 g of which was stirred with 1.6 g 1-benzylpiperazine in MeCN, then hydrolyzed with aqueous NaOH to give 1.0 g 2-(R)-(4-benzylpiperazinyl)propionic acid (II). Then, 24.5 g N-benzyloxycarbonyl-O1-ethyl-D-glutamic acid was stirred with 17.5 g Et (2S, 3aS, 7aS)-octahydro-1H-indole-2-carboxylate-HCl in CH2Cl2, then reduced,and then hydrolyzed with aqueous NaOH to give 15.01 g (2S, 3aS, 7aS)-1-(γ-D-glutamyl)octahydro-1H-indole-2-carboxylic acid (III). Then, 0.8 g II was treated with 0.4 g N-hydroxysuccinimide in CHCl3 to give 2-(R)-(4-benzylpiperazinyl)propionic acid N-hydroxysuccinimide ester, which was treated with 1.0 g III in THF to give 0.8 g (2S, 3aS, 7aS)-1-[N-2(R)-(4-benzylpiperazinyl)propionyl]-γ-D-glutamyl]octahydro-1H-indole-2-carboxylic acid, 0.4 g of which was refluxed with HCO2H in MeOH in the presence of Pd black for 4 h to give 0.2 g (2S, 3aS, 7aS)-1-[N-(2R)-piperazinylpropionyl)-γ-D-glutamyl]octahydro-1H-indole-2-carboxylic acid, which showed an IC50 of 2.1 + 10-7 M against angiotensin converting enzyme.

IT **124078-64-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation of, with (glutamyl)indolecarboxylic acid)

RN 124078-64-4 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[1-oxo-2-[4-(phenylmethyl)-1-piperazinyl]propoxy]-, (R)- (9CI) (CA INDEX NAME)

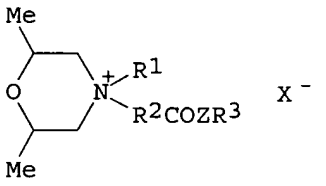
Absolute stereochemistry.



L8 ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:589581 HCAPLUS
DOCUMENT NUMBER: 111:189581
TITLE: Morpholinoalkylcarboxylates as plant growth regulators and fungicides
INVENTOR(S): Ballschuh, Detlef; Banasiak, Lothar; Gruenzel, Hermann; Kluge, Eberhard; Lyr, Horst; Ohme, Roland; Rusche, Jochen; Seibt, Horst; Spengler, Dieter; Stoeckel, Christian
PATENT ASSIGNEE(S): Akademie der Landwirtschaftwissenschaften der DDR, Institut fuer Pflanzenschutzforschung, Ger. Dem. Rep.
SOURCE: Ger. (East), 28 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 263688	A1	19890111	DD 1985-278326	19850705

PRIORITY APPLN. INFO.: DD 1985-278326 19850705
OTHER SOURCE(S): MARPAT 111:189581
GI



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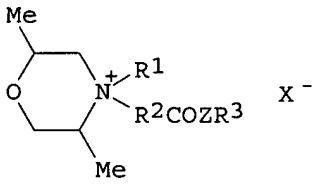


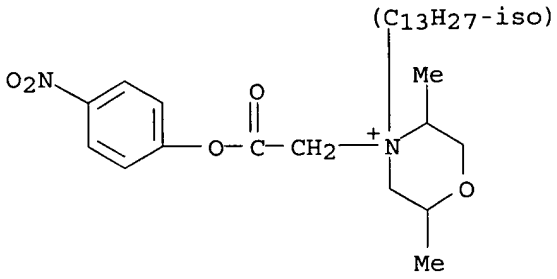
II

AB Mixts. of the title compds. I and II [R1 = C6-20; R2 = C1-6 alkylene; R3 = (un)substituted alkyl, alkenyl, cycloalkyl, etc.; Z = O, S; X- = anion]

(cis and/or trans) are prepared as fungicides and plant growth regulators. The fungicidal activity is both curative and preventive. Many target fungal species and host plants are listed. A mixture of cis- and/or trans-2,5-dimethyl-N-isotridecylmorpholine and cis- and/or trans-2,6-dimethyl-N-isotridecylmorpholine was refluxed with ClCH2CO2Me in NaI-containing acetonitrile, to give I-II (R1 = isotridecyl, R2 = CH2, R3 = Me, Z = O, X = Cl).

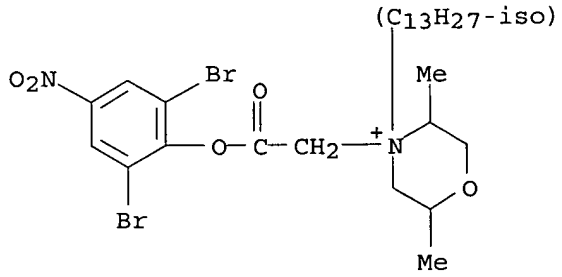
IT **123322-75-8P 123322-78-1P 123340-64-7P 123340-67-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as fungicide and plant growth regulator)

RN 123322-75-8 HCAPLUS
CN Morpholinium, 4-isotridecyl-2,5-dimethyl-4-[2-(4-nitrophenoxy)-2-oxoethyl]-, chloride (9CI) (CA INDEX NAME)



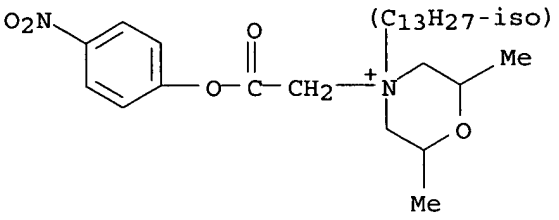
● Cl⁻

RN 123322-78-1 HCAPLUS
CN Morpholinium, 4-[2-(2,6-dibromo-4-nitrophenoxy)-2-oxoethyl]-4-isotridecyl-2,5-dimethyl-, chloride (9CI) (CA INDEX NAME)



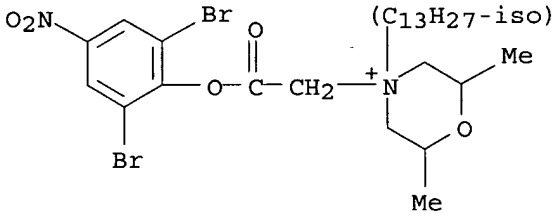
● Cl⁻

RN 123340-64-7 HCAPLUS
CN Morpholinium, 4-isotridecyl-2,6-dimethyl-4-[2-(4-nitrophenoxy)-2-oxoethyl]-, chloride (9CI) (CA INDEX NAME)



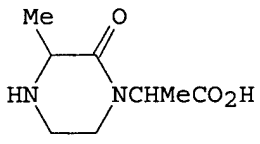
● Cl⁻

RN 123340-67-0 HCAPLUS
CN Morpholinium, 4-[2-(2,6-dibromo-4-nitrophenoxy)-2-oxoethyl]-4-isotridecyl-2,6-dimethyl-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L8 ANSWER 22 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:423356 HCAPLUS
DOCUMENT NUMBER: 109:23356
TITLE: Interactions of organic substrates with 30- and 36-membered ring peptides containing (2S,3'S)-2-(2'-oxo-3'-methylpiperazin-1'-yl)propanoic acid and sarcosine
AUTHOR(S): Kojima, Yoshitane; Yamashita, Tetsushi; Shibata, Kozo; Ohsuka, Akio
CORPORATE SOURCE: Fac. Sci., Osaka City Univ., Osaka, 558, Japan
SOURCE: Polymer Journal (Tokyo, Japan) (1987), 19(10), 1221-3
CODEN: POLJB8; ISSN: 0032-3896
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Synthetic routes to cyclic peptides cyclo(Sar-EAA)4 (EAA = residue of title acid I) and cyclo(Sar-Sar-Sar-EAA)2 are described. Interaction of these cyclic peptides with p-toluenesulfonic acid salt of sodium, benzylamine, and 4-phenylbutylamine were studied by 1H NMR.

IT **114967-10-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

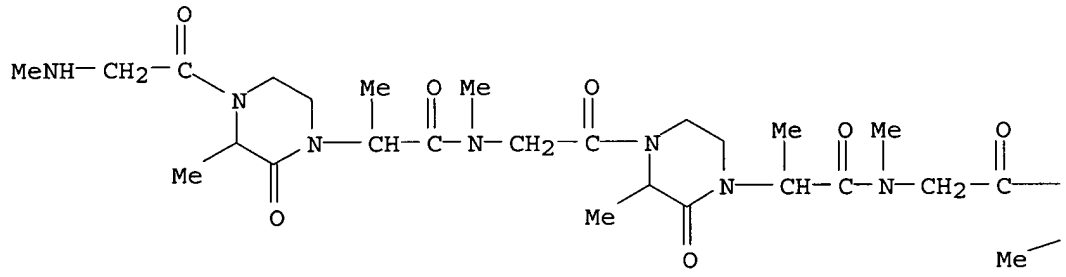
RN 114967-10-1 HCAPLUS

CN 1-Piperazineacetamide, N-[2-[4-[2-[[2-[4-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1-methyl-2-oxoethyl]-2-methyl-3-oxo-1-piperazinyl]-2-oxoethyl]methylamino]-1-methyl-2-oxoethyl]-2-methyl-3-oxo-1-piperazinyl]-2-oxoethyl]-N,α,3-trimethyl-4-[[methyl[2-[3-methyl-4-[(methylamino)acetyl]-2-oxo-1-piperazinyl]-1-oxopropyl]amino]acetyl]-2-oxo-, [3S-[1[R*[R*[R*[R*(R*)]]]],3R*,4[R*(R*)]]]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

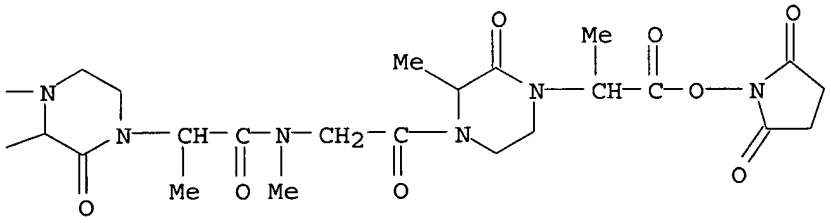
CM 1

CRN 114967-09-8
CMF C48 H73 N13 O15

PAGE 1-A

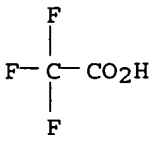


PAGE 1-B

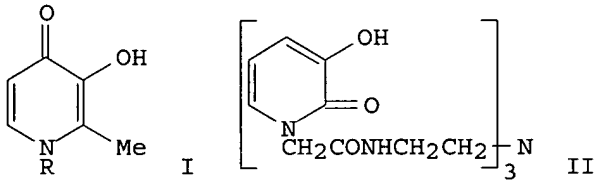


CM 2

CRN 76-05-1
CMF C2 H F3 O2



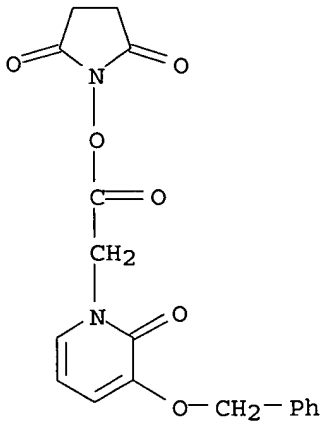
L8 ANSWER 23 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:49290 HCAPLUS
DOCUMENT NUMBER: 108:49290
TITLE: In vivo evaluation of hydroxypyridone iron chelators in a mouse model
AUTHOR(S): Gyparaki, M.; Porter, J. B.; Streater, M.; Hider, R. C.; Huehns, E. R.
CORPORATE SOURCE: Dep. Haematol., Univ. Coll. London, London, WC1 E6HX, UK
SOURCE: Acta Haematologica (1987), 78(3), 217-21
CODEN: ACHAAH; ISSN: 0001-5792
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Six N-substituted 3-hydroxypyrid-4-ones (I; R = Me, Et, Pr, iso-Pr, Bu, or hexyl) caused excretion when given i.p. to Fe-overloaded mice. The 1st 5 I were also active when given orally. Based on considerations of toxicity and relative activity, the compds. most promising for clin. use appeared to be I (R = Et) and I (R = Pr). A hexadentate pyrid-2-one (II) also caused Fe excretion when given i.p. or orally.

IT **95215-73-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tris(aminoethyl)amine)

RN 95215-73-9 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)

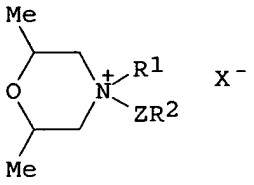


L8 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:156487 HCAPLUS
DOCUMENT NUMBER: 106:156487
TITLE: Salts of morpholinocarboxylic esters and morpholinoalkyl phenyl ethers, processes for their preparation, and their use as fungicides and plant growth regulators.
INVENTOR(S): Banasiak, Lothar; Leuner, Brita; Lyr, Horst; Nega, Eva; Sunkel, Marianne
PATENT ASSIGNEE(S): Institut fuer Pflanzenschutzforschung Kleinmachnow, Ger. Dem. Rep.
SOURCE: Eur. Pat. Appl., 41 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 209763	A1	19870128	EP 1986-108916	19860701
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
DD 263685	A1	19890111	DD 1985-278323	19850705
DD 263687	A1	19890111	DD 1985-278325	19850705
AU 8659401	A1	19870108	AU 1986-59401	19860630
DK 8603151	A	19870106	DK 1986-3151	19860702
FI 8602851	A	19870106	FI 1986-2851	19860704
ZA 8605002	A	19870325	ZA 1986-5002	19860704
JP 62084065	A2	19870417	JP 1986-156349	19860704
HU 42288	A2	19870728	HU 1986-2826	19860704
HU 42286	A2	19870728	HU 1986-2827	19860704
ES 2001853	A6	19880701	ES 1986-125	19860704
PL 146362	B1	19890131	PL 1986-260474	19860704
CS 264279	B2	19890613	CS 1986-5135	19860707

PRIORITY APPLN. INFO.: DD 1985-278323 A 19850705
DD 1985-278325 A 19850705

GI



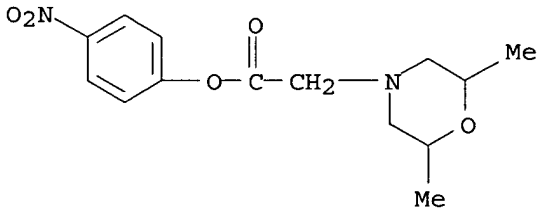
I

AB The title compds. [I; R = C6-20 alkyl; R2 = R3Z1CO, (un)substituted PhO; R3 = (halo)alkenyl, alkynyl, (un)substituted alkyl, cycloalkyl, aryl, aralkyl; X1 = anion of a nonphytotoxic acid; Z = O, S; Z1 = C1-6 alkylene; R3 and X- may be absent] were prepared as fungicides and plant growth regulators. A mixture of 30 g 4-isotridecyl-2,6-dimethylmorpholine and 10.9 g ClCH2CO2Me was refluxed 20 h in MeCN containing catalytic NaI to give 38 g I (R1 = isotridecyl, R2 = CO2Me, X = Cl, Z = CH2)(II). At 10 μg/mL II gave 88% inhibition of growth of Botrytis cinerea. At 1000 mg/L II reduced the growth of cucumber plants by 32%.

IT **107562-00-5DP**, quaternary derivs. **107562-11-8DP**, quaternary derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as fungicide and plant growth inhibitor)

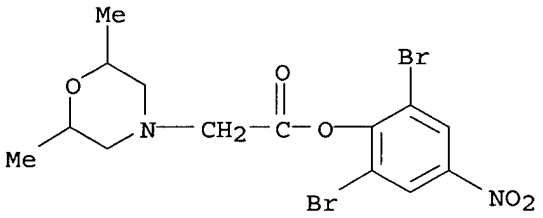
RN 107562-00-5 HCAPLUS

CN 4-Morpholineacetic acid, 2,6-dimethyl-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



RN 107562-11-8 HCAPLUS

CN 4-Morpholineacetic acid, 2,6-dimethyl-, 2,6-dibromo-4-nitrophenyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:596001 HCAPLUS

DOCUMENT NUMBER: 103:196001

TITLE: Hydroxypyridinone derivatives and pharmaceutical compositions containing them

INVENTOR(S): Hider, Robert Charles; Kontoghiorghes, George; Silver,

Jack; Stockham, Michael Arthur
PATENT ASSIGNEE(S): National Research Development Corp., UK
SOURCE: Eur. Pat. Appl., 55 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 138421	A2	19850424	EP 1984-306438	19840920
EP 138421	A3	19870603		
EP 138421	B1	19901205		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4666927	A	19870519	US 1984-651684	19840918
GB 2146989	A1	19850501	GB 1984-23799	19840920
GB 2146989	B2	19870218		
ZA 8407408	A	19860528	ZA 1984-7408	19840920
EP 357150	A1	19900307	EP 1989-202213	19840920
EP 357150	B1	19931208		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
DK 8404536	A	19850324	DK 1984-4536	19840921
DK 158349	B	19900507		
DK 158349	C	19901015		
JP 60094965	A2	19850528	JP 1984-201408	19840925
JP 06002739	B4	19940112		
US 4863913	A	19890905	US 1986-944355	19861222
US 4912118	A	19900327	US 1986-944872	19861222
US 5104865	A	19920414	US 1989-403054	19890901
JP 02191254	A2	19900727	JP 1989-324877	19891212
JP 06002740	B4	19940112		

PRIORITY APPLN. INFO.:

GB 1983-25494	A	19830923
US 1984-651684	A	19840918
EP 1984-306438	P	19840920
US 1986-944355	B1	19861222

OTHER SOURCE(S): CASREACT 103:196001

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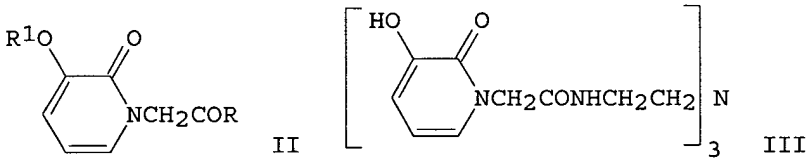


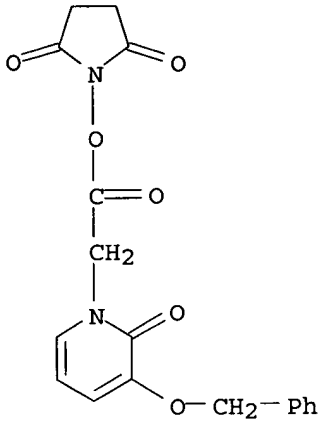
AB Title compds. (I) were prepared, in which two or more 3-hydroxypyrid-2-one, 3-hydroxypyrid-4-one, or 1-hydroxypyrid-2-one rings are linked. Thus, 2,3-dihydroxypyridine and EtO2CCH2Br reacted to give hydroxypyridone II (R = OEt, R1 = H), which reacted with PhCH2Cl-NaOH to give 41% II (R = OH, R1 = CH2Ph). Treatment of the latter compound with DCC and N-hydroxysuccinimide gave 80% 1-succinimido ester, which condensed with N(CH2CH2NH2)3 to give, after hydrogenolysis, 68% triamide III. III removed 40% of iron from 59Fe(III)-loaded human transferrin, vs. 27% for EDTA. Addnl., the accumulation of the Fe(III) complex of III in human

erythrocytes was >9-fold that of Fe(III) citrate.

IT **95215-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of)

RN 95215-73-9 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1985:487778 HCAPLUS

DOCUMENT NUMBER: 103:87778

TITLE: N-(1,2-Diacyl-2-halo-1-vinyl)pyridinium salts

INVENTOR(S): Richter, Andreas M.; Fanghaenel, Egon

PATENT ASSIGNEE(S): Technische Hochschule "Carl Schorlemmer" Leuna-Merseburg, Ger. Dem. Rep.

SOURCE: Ger. (East), 7 pp.
CODEN: GEXXA8

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DD 215308	A1	19841107	DD 1983-251654	19830602

PRIORITY APPLN. INFO.: DD 1983-251654 19830602

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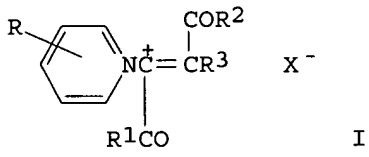


I

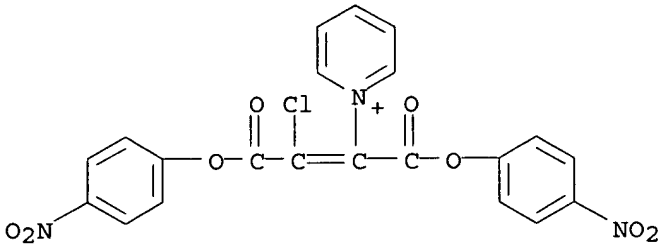
AB Title compds. I (R = H, alkyl, alkoxy, dialkylamino; R1, R2 = alkyl, aralkyl, aryl, alkoxy, aralkoxy, aryloxy, alkylthio, aralkylthio, arylthio; R3 = F, Cl, Br, iodo; X- = halide, ClO4-, BF4-) were prepared by

reacting R1COC.tplbond.CCOR2 with halogen and (un)substituted pyridines (II); or by reacting R1COCR4:CR5COR2 (R4, R5 = F, Cl, Br, iodo) with II; or by reacting R6COCR7:CR8COR9 (R6-R9 = F, Cl, Br, iodo) with R1OH or R1SH and II. Thus, 4-O2NC6H4O2CCCl:CClCO2C6H4NO2-4 was treated with pyridine to give 99% I (R = H, R1 = R2 = 4-O2NC6H4O, R3 = Cl, X = Cl). I are useful as intermediates in the preparation of dyes, heterocycles, polymers, and biol. active substances.

IT **97683-50-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 97683-50-6 HCAPLUS

CN Pyridinium, 1-[2-chloro-3-(4-nitrophenoxy)-1-[(4-nitrophenoxy)carbonyl]-3-oxo-1-propenyl]-, chloride (9CI) (CA INDEX NAME)

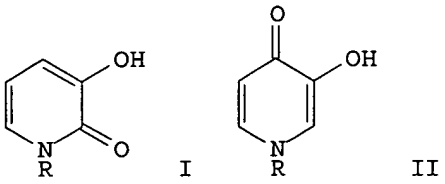


● Cl^-

L8 ANSWER 27 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:113302 HCAPLUS
DOCUMENT NUMBER: 102:113302
TITLE: Iron complexes for pharmaceutical compositions
INVENTOR(S): Hider, Robert Charles; Kontoghiorghes, George; Silver, Jack; Stockham, Michael Arthur
PATENT ASSIGNEE(S): National Research Development Corp., UK
SOURCE: Brit. UK Pat. Appl., 19 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2136806	A1	19840926	GB 1984-7180	19840320
GB 2136806	B2	19870415		
EP 120670	A1	19841003	EP 1984-301882	19840320
EP 120670	B1	19881221		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4650793	A	19870317	US 1984-592543	19840322
DK 8401659	A	19840925	DK 1984-1659	19840323
DK 159305	B	19901001		
DK 159305	C	19910304		
JP 59181258	A2	19841015	JP 1984-57186	19840324
JP 06025120	B4	19940406		
US 36831	E	20000822	US 1995-390588	19950217
PRIORITY APPLN. INFO.:			GB 1983-8055 A	19830324

US 1984-592543 A5 19840322
OTHER SOURCE(S): CASREACT 102:113302; MARPAT 102:113302
GI

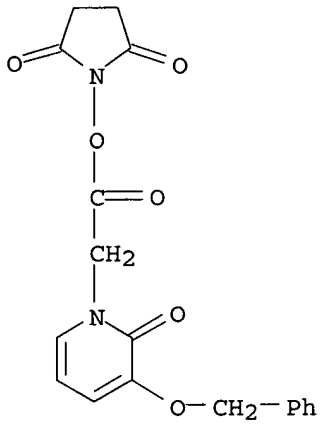


I II

AB Fe complexes of 3-hydroxy-2- and -4-pyridones I and II [R = acyl, (un)substituted hydrocarbon], useful for treatment of Fe deficiency anemia, were prepared Thus 2,3-dihydroxypyridine was treated with AcBr to give I (R = Ac), which complexed Fe(III) to give FeL3 (L = I; R = Ac) (III). Fe uptake from III by rat jejunal sacs in vitro was 38 times greater than from FeCl3.

IT **95215-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of, with amines)

RN 95215-73-9 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 28 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:113301 HCAPLUS
DOCUMENT NUMBER: 102:113301
TITLE: Pharmaceutical compositions
INVENTOR(S): Hider, Robert Charles; Kontoghiorghes, George; Silver, Jack
PATENT ASSIGNEE(S): National Research Development Corp., UK
SOURCE: Brit. UK Pat. Appl., 17 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2136807	A1	19840926	GB 1984-7181	19840320
GB 2136807	B2	19870423		
CA 1243606	A1	19881025	CA 1984-446932	19840207
EP 120669	A2	19841003	EP 1984-301881	19840320
EP 120669	A3	19850123		
EP 120669	B1	19910123		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
EP 305646	A2	19890308	EP 1988-107000	19840320
EP 305646	A3	19900808		
EP 305646	B1	19961113		
R: BE, CH, DE, FR, GB, IT, LI, NL, SE				
US 4585780	A	19860429	US 1984-592271	19840322
JP 59205361	A2	19841120	JP 1984-57185	19840324
JP 06072097	B4	19940914		
CA 1338496	A1	19960730	CA 1986-524044	19861128
JP 06080637	A2	19940322	JP 1993-150865	19930622
JP 07064815	B4	19950712		
US 35948	E	19981103	US 1995-397321	19950217

PRIORITY APPLN. INFO.:

GB 1983-8054	A	19830324
CA 1984-446932	A3	19840207
EP 1984-301881	P	19840320
US 1984-592271	A5	19840322

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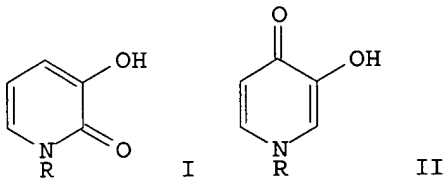
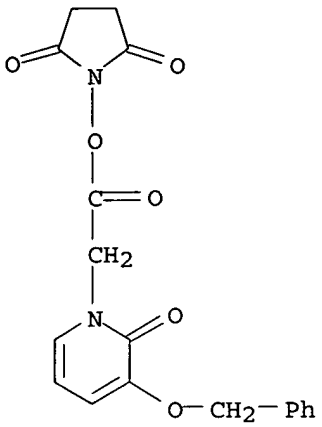


AB N-Substituted 3-hydroxy-2- or -4-pyridones I and II [R = acyl, (un)substituted hydrocarbon], useful for Fe complexation in vivo in treating Fe overloads, were prepared Thus 2,3-dihydroxypyridine was treated with AcBr to give hydroxy-2-pyridone I (R = Ac) (III). At 10 mg/mouse intragastrically, III gave 137 ± 45% excretion of 59Fe lactoferrin in Fe-loaded mice, compared to blank controls.

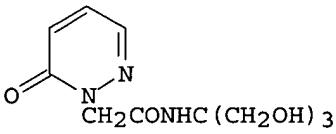
IT **95215-73-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of, with amines)

RN 95215-73-9 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[2-oxo-3-(phenylmethoxy)-1(2H)-pyridinyl]acetyl]oxy]- (9CI) (CA INDEX NAME)



L8 ANSWER 29 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:113157 HCAPLUS
DOCUMENT NUMBER: 102:113157
TITLE: Preparation and biological effects of N-[tris(hydroxymethyl)methylaminocarbonylmethyl] derivatives of heterocyclic bases
AUTHOR(S): Pischel, Helmut; Holy, Antonin; Vesely, Jiri; Wagner, Guenther
CORPORATE SOURCE: Sekt. Biowiss.-Pharm., Karl-Marx-Univ., Leipzig, Ger. Dem. Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (1984), 49(11), 2541-50
CODEN: CCCCAK; ISSN: 0366-547X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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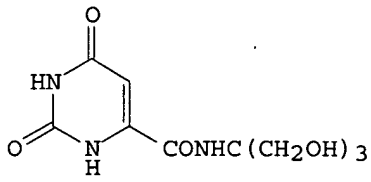
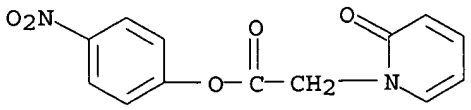


II

AB The title compds. were synthesized by the reaction of (HOCH2)3CNH2 with p-nitrophenyl or alkyl esters of N-carboxymethyl derivs. of uracil, 5-chloro-, 5-bromo-, 5-iodouracil, thymine, cytosine, 6-azauracil, 2-pyridone, 2-pyrimidone, 3-pyridazone and orotic acid. Some novel intermediates were also prepared Of all the amides tested, only the 3-pyridazone derivative I and orotic acid derivative II inhibited the growth of L-1210 mouse leukemic cells in vitro with ID50 .apprx.10-4 mol l-1.
IT **95209-96-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with TRIS)
RN 95209-96-4 HCAPLUS
CN 1(2H)-Pyridineacetic acid, 2-oxo-, 4-nitrophenyl ester (9CI) (CA INDEX

NAME)



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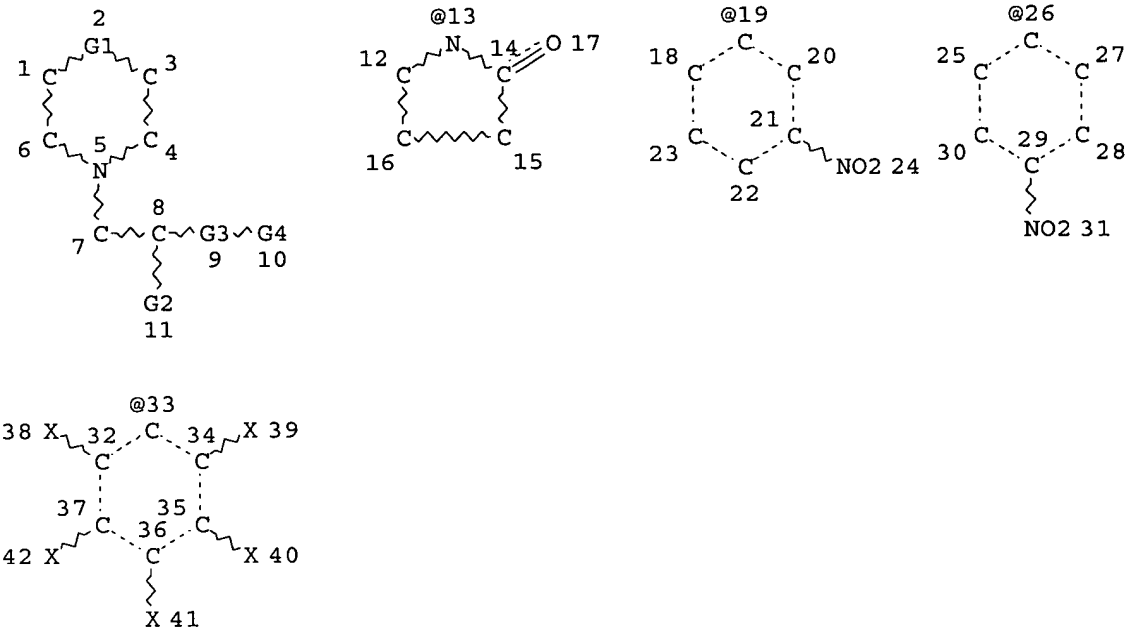

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VAR G3=O/S
VAR G4=13/19/26/33
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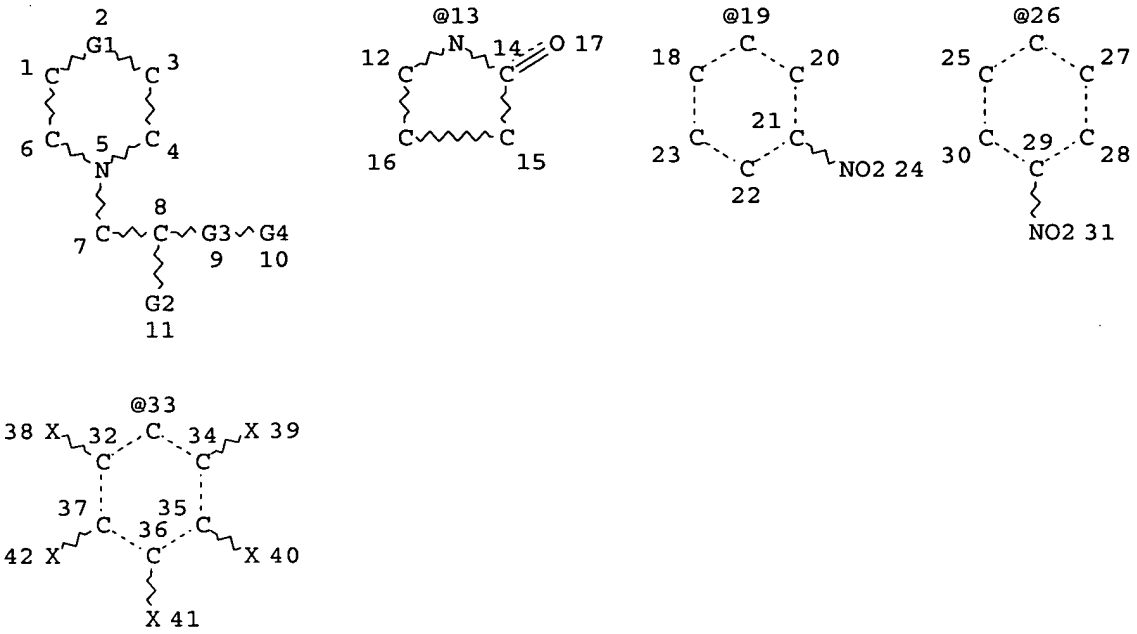
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L5 82 SEA FILE=REGISTRY SSS FUL L1
L6 STR



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VAR G2=O/S/N
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VAR G4=13/19/26/33
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L7 46 SEA FILE=REGISTRY SUB=L5 SSS FUL L6
L8 29 SEA FILE=HCAPLUS ABB=ON PLU=ON L7
L9 36 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L7
L10 18 SEA FILE=HCAPLUS ABB=ON PLU=ON L9
L11 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT L8

=> d ibib abs hitstr l11 1-17

L11 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:399339 HCAPLUS
DOCUMENT NUMBER: 141:254556
TITLE: Grassland's locoweed toxin vaccine
INVENTOR(S): Dong, Dewen; Cao, Guangrong; Zhao, Baoyu; Ge, Pengbin
PATENT ASSIGNEE(S): Danong Biotechnology Co., Ltd., Yangling, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 17 pp. CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1395967	A	20030212	CN 2002-114592	20020524

PRIORITY APPLN. INFO.: CN 2002-114592 20020524

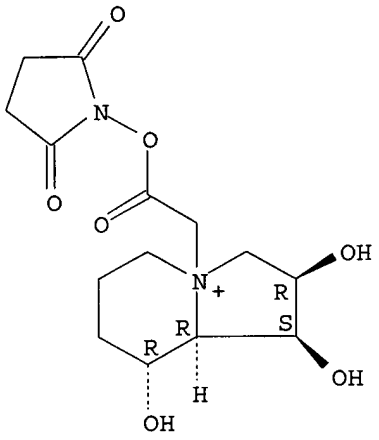
AB The process comprises N-alkylating swainsonine with bromoacetic acid N-succinimido ester in acetone under refluxing, coupling with bovine serum albumin in water at 0 °C, dialyzing, freeze drying, and emulsifying with Freund's adjuvant.

IT **754196-04-8P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vaccine for Grassland's locoweed toxin)

RN 754196-04-8 HCAPLUS

CN Indolizinium, 4-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]octahydro-1,2,8-trihydroxy-, bromide, (1S,2R,8R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br^-

L11 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:913165 HCAPLUS
DOCUMENT NUMBER: 139:381472
TITLE: Preparation of naphthaldiimide derivatives as anti-Helicobacter agents
INVENTOR(S): Sugimori, Giichi; Masui, Moriyasu; Nishida, Kuniyoshi; Hasegawa, Yasushi; Kobayashi, Naotake
PATENT ASSIGNEE(S): Shionogi & Co., Ltd., Japan
SOURCE: PCT Int. Appl., 157 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003095453	A1	20031120	WO 2003-JP5795	20030508

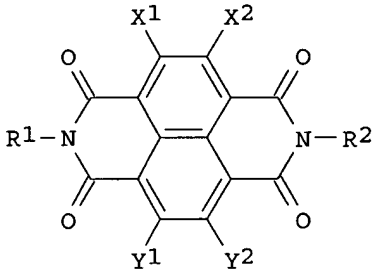
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003235908	A1	20031111	AU 2003-235908		20030508
PRIORITY APPLN. INFO.:			JP 2002-137845	A	20020513
			WO 2003-JP5795	W	20030508

OTHER SOURCE(S): MARPAT 139:381472

GI



I

AB Title compds. I (R1, R2 = H, alkyl, cycloalkyl, heterocyclyl, etc; X1, X2, Y1, Y2 = H, halo, etc.) are prepared When employed alone, such a compound is useful as an agent against Helicobacter. When employed as a combined drug, it can remarkably lessen side effects occurring in treating digestive ulcer, etc. These compds. or compns. can specifically injure and remove Helicobacter to thereby effectively treat digestive diseases (for example, gastric ulcer, duodenal ulcer, gastritis and gastric cancer).

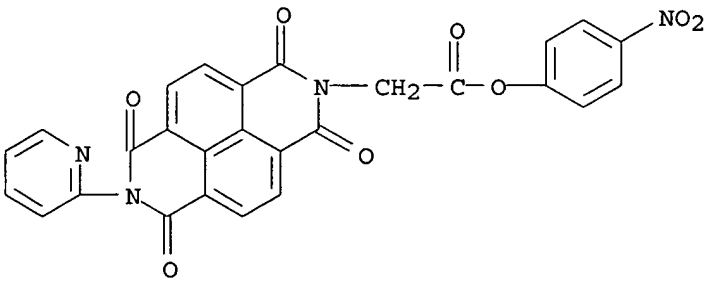
IT **625085-55-4P 625086-14-8P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

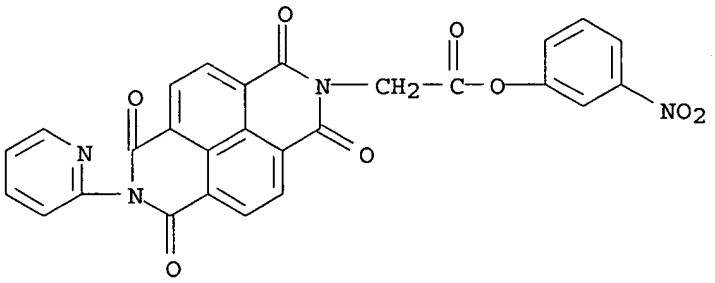
(preparation of naphthaldiimide derivs. as anti-Helicobacter agents)

RN 625085-55-4 HCAPLUS

CN Benzo[lmn][3,8]phenanthroline-2(1H)-acetic acid, 3,6,7,8-tetrahydro-1,3,6,8-tetraoxo-7-(2-pyridinyl)-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



RN 625086-14-8 HCAPLUS
CN Benzo[lmn][3,8]phenanthroline-2(1H)-acetic acid, 3,6,7,8-tetrahydro-1,3,6,8-tetraoxo-7-(2-pyridinyl)-, 3-nitrophenyl ester (9CI) (CA INDEX NAME)

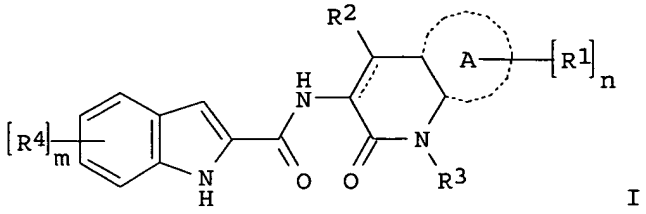


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:719471 HCAPLUS
DOCUMENT NUMBER: 139:261174
TITLE: Preparation of N-heterocyclyl indole-2-carboxamides as glycogen phosphorylase inhibitors
INVENTOR(S): Birch, Alan Martin; Morley, Andrew David
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003074513	A2	20030912	WO 2003-GB893	20030304
WO 2003074513	A3	20031231		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003216991	A1	20030916	AU 2003-216991	20030304
EP 1485371	A2	20041215	EP 2003-712313	20030304
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005131016	A1	20050616	US 2003-506748	20030304
JP 2005525364	T2	20050825	JP 2003-572981	20030304
PRIORITY APPLN. INFO.:			GB 2002-5162 A	20020306
			WO 2003-GB893 W	20030304

OTHER SOURCE(S): MARPAT 139:261174
GI



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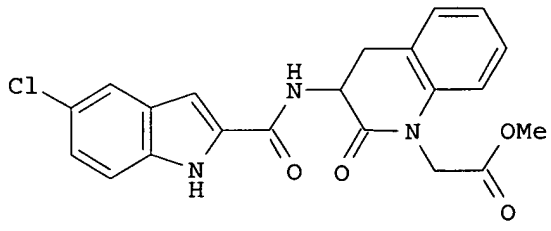


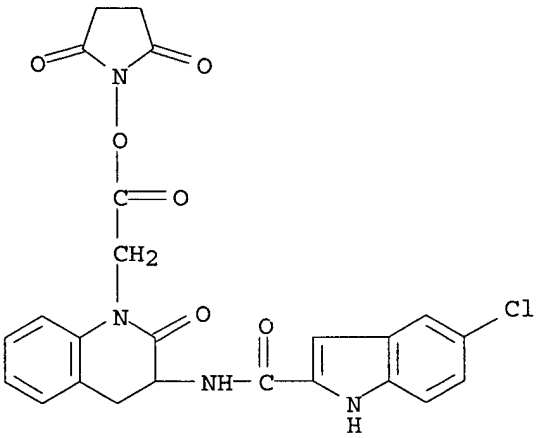
II

AB The title compds. [I; A = phenylene or heteroarylene; m = 0-2; n = 0-2; R1 = halo, NO2, CN, OH, CO2H, etc.; R2 = H, OH, CO2H; R3 = H, OH, aryl, heterocyclyl, etc.; R4 = H, halo, NO2, CN, etc.] which possess glycogen phosphorylase inhibitory activity and accordingly have value in the treatment of disease states associated with increased glycogen phosphorylase activity such as diabetes type II, were prepared Thus, amidation of 5-chloro-1H-indole-2-carboxylic acid with Me 2-(3-amino-2-oxo-3,4-dihydroquinolin-1-(2H)-yl)acetate (preparation given) in the presence of HOBT, DCM and EDCI afforded 59% II. The compds. I showed IC50 values in the range 100μM to 1nM against against hrl glycogen phosphorylase a. Pharmaceutical composition comprising the compound I was claimed.

IT **599193-13-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-heterocyclyl indole-2-carboxamides as glycogen phosphorylase inhibitors)

RN 599193-13-2 HCAPLUS

CN 1H-Indole-2-carboxamide, 5-chloro-N-[1-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-1,2,3,4-tetrahydro-2-oxo-3-quinolinyl]- (9CI) (CA INDEX NAME)

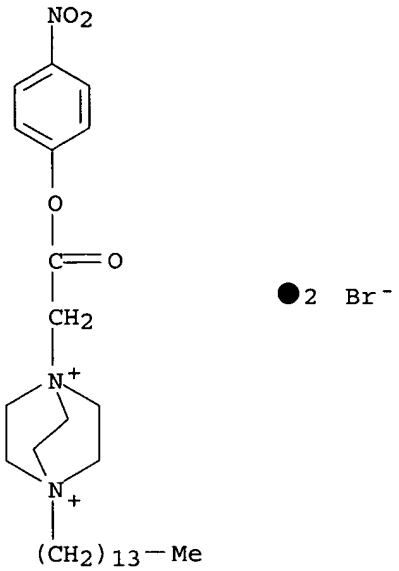


L11 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:575812 HCAPLUS
DOCUMENT NUMBER: 137:381573
TITLE: Chemical Ribonucleases: 4.1 An Analysis of the Domain Structure of Chemical Ribonucleases Based on 1,4-Diazabicyclo[2.2.2]octane
AUTHOR(S): Konevetz, D. A.; Mironova, N. L.; Beck, I. E.; Zenkova, M. A.; Shishkin, G. V.; Vlassov, V. V.; Silnikov, V. N.
CORPORATE SOURCE: Novosibirsk Institute of Bioorganic Chemistry, Russian Academy of Sciences, Siberian Branch, Novosibirsk, 630090, Russia
SOURCE: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2002), 28(4), 331-341
CODEN: RJBCET; ISSN: 1068-1620
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:381573

AB Artificial RNases of the ABLkCm series were synthesized. They consist of a lipophilic alkyl radical (Et, n-C14H29, or n-C15H31) [Acy], an "RNA-binding domain" [Vcy] (bisquaternary salt of 1,4-diazabicyclo[2.2.2]octane), a "catalytic domain" [Scy]m [histamine ([Scy]1) or histidine ([Scy]3) residue], and a "linker" Lk that joins the "domains" B and Cm [here, k is the number of methylene units (one or three) in the linker]. The effect of the "domain structure" on the catalytic properties of the chemical RNases was analyzed using seven compds. of this series (ABL1C1, ABL3C1, ABL3C3, AC1, AB, BL2, and BL3C3). The catalytic activity of the compds. was assessed in the reaction of hydrolysis of the in vitro transcripts of human tRNALys and yeast tRNAAsp under physiol. conditions. It was shown that only chemical RNases that involve all the fragments of the ABLkCm construct can hydrolyze the substrate tRNA at a high rate (90% of tRNA is hydrolyzed for 10 h at 37° [Scy]). The activity of the compds. is largely determined by the presence of a long lipophilic radical linked to 1,4-diazabicyclo[2.2.2]octane and a long linker, which joins the RNA-hydrolyzing and RNA-binding domains. The results indicate an important role of hydrophobic interactions in the acceleration of the RNA hydrolysis reaction.

IT **475661-85-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(all domains of chemical RNase are required for efficient tRNA hydrolysis)
RN 475661-85-9 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-[2-(4-nitrophenoxy)-2-oxoethyl]-4-tetradecyl-, dibromide (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:504749 HCAPLUS
DOCUMENT NUMBER: 137:79227
TITLE: Novel functional peptide nucleic acid monomer and process for producing the same
INVENTOR(S): Ikeda, Hisafumi; Saito, Isao; Kitagawa, Fumihiko
PATENT ASSIGNEE(S): Applied Biosystems Japan Ltd., Japan
SOURCE: PCT Int. Appl., 63 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002051797	A1	20020704	WO 2001-JP8120		20010919
W: JP, US					
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR					
EP 1357112	A1	20031029	EP 2001-970133		20010919
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR					
US 2004101839	A1	20040527	US 2003-250592		20031224
PRIORITY APPLN. INFO.:			JP 2000-394669	A	20001226
			WO 2001-JP8120	W	20010919

OTHER SOURCE(S): CASREACT 137:79227; MARPAT 137:79227
GI

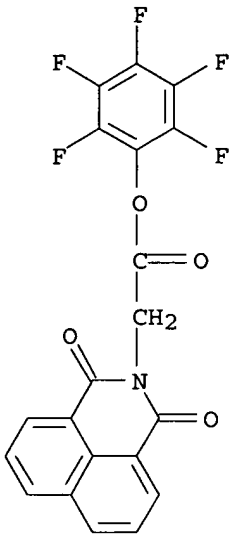
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A peptide nucleic acid (PNA) monomer represented by the following general formula A-(CH2)nCO-B [I; wherein A = Q or Q1 (wherein X = OH, Z = O; X = NH2, Z = H2N+; or X = NMe2, Z = Me2N+), Q2, Q3, Q4 (wherein R = hydrogen, NO2, NH2, NHCbz, bromine, fluorine, chlorine, or SO3Na2), Q5, 3-(4-dimethylaminophenylazo)phenyl, 4-(4-dimethylaminophenylazo)phenylsulfonylamino, 2-(4-hydroxyphenylazo)benzoylamino, 5-dimethylaminonaphthalenesulfonylamino, 1-pyrenecarbonyl, 1-pyrenylmethyl, 1-pyrenesulfonylamino, 6,7,8-trimethyl-1,3-dioxo-2,5-dihydro-2,4-diazaphenazin-2-yl, 4-methylcoumarin-7-ylaminocarbonyl, 4-trifluoromethylcoumarin-7-ylaminocarbonyl, 4-methyl-2-oxo-1,2-dihydroquinoin-7-ylaminocarbonyl, 2-oxo-1,2-dihydroquinoin-3-ylaminocarbonyl, etc.; B is OH, pentafluorophenyloxy, succinimidyloxy, N-carboxylmethyl-N-[2-(tert-butoxycarbonylamino)ethyl]amino; n = an integer of 1 to 4] is prepared A PNA monomer I [A, N = same as above; B = N-carboxylmethyl-N-[2-(tert-butoxycarbonylamino)ethyl]amino] is prepared by amidation of an active ester I (A, n = same as above; B = pentafluorophenyloxy, succinimidyloxy) with tert-butoxycarbonylaminoethylamine or an ω-amino acid derivative, in particular 2-[N-[2-(tert-butoxycarbonylamino)ethyl]amino]acetic acid (II). This process is convenient for the preparation of a photofunctional PNA monomer which is unstable under alkali condition. Thus, to a solution of 100 mg 2-(5,7,8-trimethyl-1,3-dioxo-2,5-dihydro-2,4-diazaphenazin-2-yl)acetic acid and 70.2 mg pentafluorophenol in 10 mL DMF was added 73.2 mg 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC) at 0° and stirred at 0° for 1 h and at room temperature for 12 h to give 85% 2,3,4,5,6-pentafluorophenyl 2-(5,7,8-trimethyl-1,3-dioxo-2,5-dihydro-2,4-diazaphenazin-2-yl)acetate (III). To a solution of the active ester III (100 mg) and 45.4 mg II in 10 mL DMF was added 36.3 μL diisopropylethylamine and stirred at room temperature for 15 h to give 85% 2-[N-[2-(tert-butoxycarbonylamino)ethyl]-2-[(5,7,8-trimethyl-1,3-dioxo-2,5-dihydro-2,4-diazaphenazin-2-yl)acetyl]amino]acetic acid.

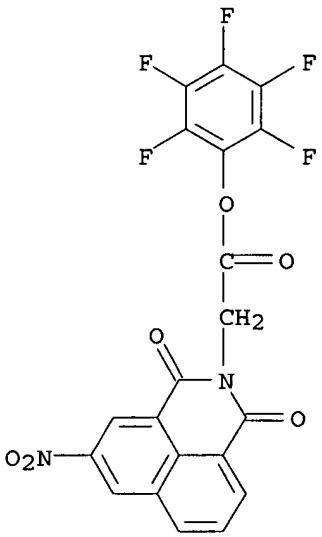
IT **439913-28-7P**, [1,3-Dioxo-1H,3H-benz[de]isoquinolin-2-yl]acetic acid pentafluorophenyl ester **439913-30-1P**, [5-Nitro-1,3-dioxo-1H,3H-benz[de]isoquinolin-2-yl]acetic acid pentafluorophenyl ester **439913-33-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel functional peptide nucleic acid monomers by amidation of active esters with α-[N-[β-(tert-butoxycarbonylamino)ethyl]amino]acetic acid.)

RN 439913-28-7 HCAPLUS

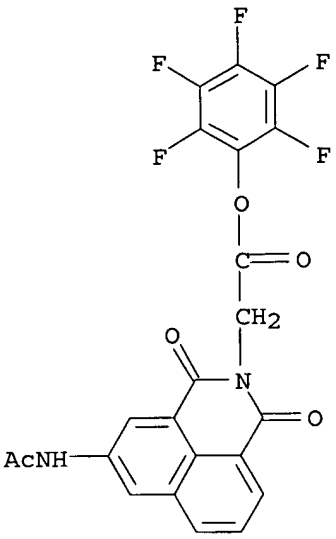
CN 1H-Benz[de]isoquinoline-2(3H)-acetic acid, 1,3-dioxo-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



RN 439913-30-1 HCAPLUS
CN 1H-Benz[de]isoquinoline-2(3H)-acetic acid, 5-nitro-1,3-dioxo-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



RN 439913-33-4 HCAPLUS
CN 1H-Benz[de]isoquinoline-2(3H)-acetic acid, 5-(acetylamino)-1,3-dioxo-, pentafluorophenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:871429 HCAPLUS
DOCUMENT NUMBER: 134:189912
TITLE: Chemical ribonucleases: 3. The synthesis of organic catalysts for the phosphodiester bond hydrolysis on the basis of quaternary salts of 1,4-diazabicyclo[2.2.2]octane
AUTHOR(S): Konevetz, D. A.; Beck, I. E.; Sil'nikov, V. N.; Zenkova, M. A.; Shishkin, G. V.
CORPORATE SOURCE: Novosibirsk Institute of Bioorganic Chemistry, Siberian Division, Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(11), 765-773
CODEN: RJBCET; ISSN: 1068-1620
PUBLISHER: MAIK Nauka/Interperiodica
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:189912

AB On the basis of imidazole and bisquaternary salts of 1,4-diazabicyclo[2.2.2]octane, a number of highly effective catalysts of the nDm series (here, n is the number of pos. charges at neutral pH values and m is the digital code of the catalytically active fragment: 1, histamine, and 2, histidine Me ester) were synthesized for the cleavage of phosphodiester bonds in ribonucleic acids. A general method for the synthesis of chemical RNases was suggested, which helps vary both the number of pos. charges in their RNA-binding domain and the catalytic center. By the example of hydrolysis under physiol. conditions of the in vitro transcript of tRNALys from human mitochondria, it was shown that the RNA cleavage rate with the nDm conjugates increases approx. 30-fold along with the increase in the number of pos. charges from two to four.

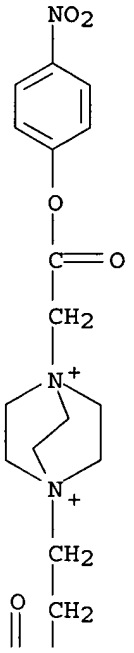
IT **327189-89-9P 327189-91-3P 327189-96-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of artificial RNases for phosphodiester bond hydrolysis of RNA

on basis of quaternary salts of 1,4-diazabicyclo[2.2.2]octane)

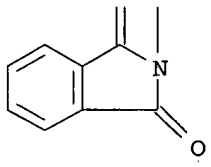
RN 327189-89-9 HCAPLUS

CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-4-[2-(4-nitrophenoxy)-2-oxoethyl]-, dibromide (9CI) (CA INDEX NAME)

PAGE 1-A



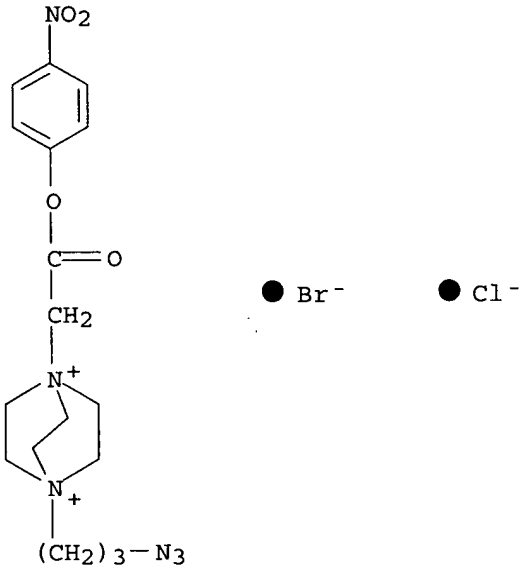
PAGE 2-A



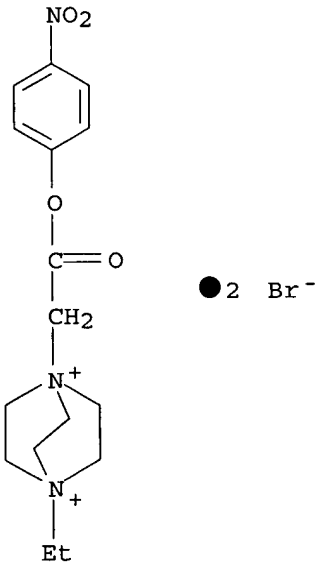
●2 Br^-

RN 327189-91-3 HCAPLUS

CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-(3-azidopropyl)-4-[2-(4-nitrophenoxy)-2-oxoethyl]-, bromide chloride (9CI) (CA INDEX NAME)



RN 327189-96-8 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-ethyl-4-[2-(4-nitrophenoxy)-2-oxoethyl]-, dibromide (9CI) (CA INDEX NAME)



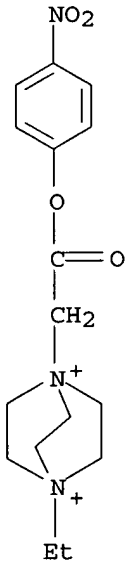
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:735652 HCAPLUS
DOCUMENT NUMBER: 133:360397
TITLE: Chemical ribonucleases: 2. Design and hydrolytic activity of the ribonuclease mimics on the basis of diazabicyclo[2.2.2]octane with a differing number of positive charges

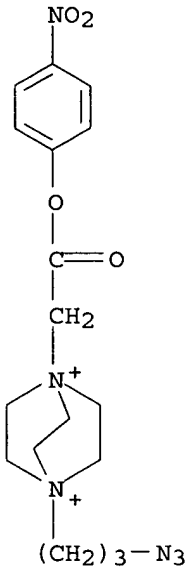
AUTHOR(S): Zenkova, M. A.; Vlassov, A. V.; Konevets, D. A.; Silnikov, V. N.; Giege, R.; Vlassov, V. V.
CORPORATE SOURCE: Novosibirsk Institute of Bioorganic Chemistry, Siberian Division, Russian Academy of Sciences, Novosibirsk, 630090, Russia
SOURCE: Russian Journal of Bioorganic Chemistry (Translation of Bioorganicheskaya Khimiya) (2000), 26(9), 610-615
CODEN: RJBCET; ISSN: 1068-1620
PUBLISHER: MAIK Nauka/Interperiodica
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A procedure was proposed allowing one to synthesize RNase mimics on the basis of conjugates of diazabicyclo[2.2.2]octane with imidazole bearing a varying number of pos. charges (nDm series, where n is the number of pos. charges at neutral pH, m is the code of an imidazole-containing fragment of the catalytic domain: 1, histamine; 2, histidine Me ester). The hydrolytic activity of six compds. of this series was studied in physiol. conditions using in vitro transcript of human mitochondrial tRNALys as a substrate. It was shown that the rate of RNA hydrolysis with nDm conjugates rises with an increase in the number of pos. charges: an approx. 30-fold acceleration of hydrolysis was observed with an increase in the total charge of the construct from +2 to +4.

IT **307305-05-1P 307305-06-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design and hydrolytic activity of RNase mimics based on diazabicyclo[2.2.2]octane and containing various number of pos. charges)

RN 307305-05-1 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-ethyl-4-[2-(4-nitrophenoxy)-2-oxoethyl]- (9CI) (CA INDEX NAME)

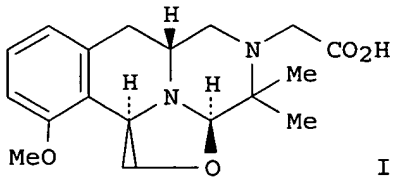


RN 307305-06-2 HCAPLUS
CN 1,4-Diazoniabicyclo[2.2.2]octane, 1-(3-azidopropyl)-4-[2-(4-nitrophenoxy)-2-oxoethyl]- (9CI) (CA INDEX NAME)

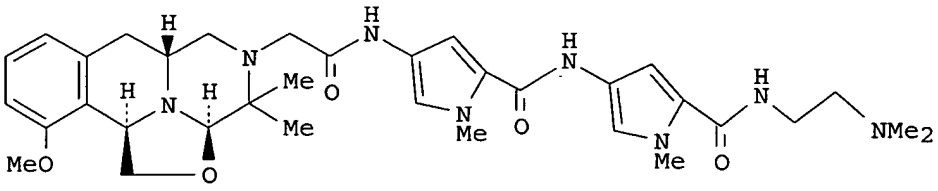


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:157026 HCAPLUS
DOCUMENT NUMBER: 133:4837
TITLE: Synthesis of a netropsin conjugate of a water-soluble epi-quinocarcin analogue: the importance of stereochemistry at nitrogen
AUTHOR(S): Herberich, B.; Scott, J. D.; Williams, R. M.
CORPORATE SOURCE: Department of Chemistry, Colorado State University, Fort Collins, CO, USA
SOURCE: Bioorganic & Medicinal Chemistry (2000), 8(3), 523-532
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

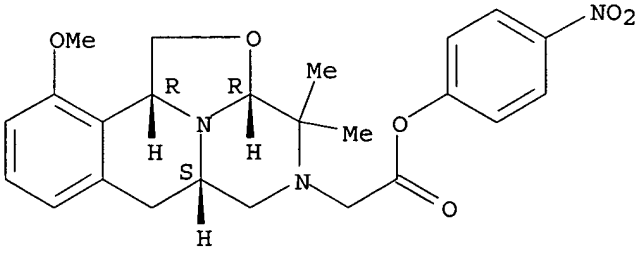
AB The efficient synthesis of a water-soluble C11a-epi-analog I of quinocarcin is described. This substance, and a netropsin amide conjugate II lack the capacity to inflict oxidative damage on DNA due to the stereoelectronic geometry of their oxazolidine nitrogen atoms. The capacity of these substances to alkylate DNA through the generation of an iminium species has been examined Both compds. were found to be unreactive as DNA alkylating agents. The results of this study are discussed in the context of previous proposals on the mode of action of this family of antitumor alkaloids.

IT **165253-50-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of a netropsin conjugate of a water-soluble epi-quinocarcin analog and the importance of stereochem. at nitrogen)

RN 165253-50-9 HCAPLUS

CN 2-Oxa-4,10c-diazaaceanthrylene-4(1H)-acetic acid, 2a,3,5,5a,6,10b-hexahydro-10-methoxy-3,3-dimethyl-, 4-nitrophenyl ester, (2aR,5aS,10bR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

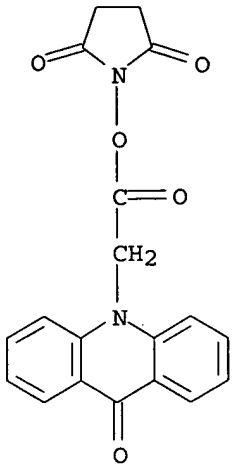
L11 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:759500 HCAPLUS
DOCUMENT NUMBER: 132:148595

TITLE: Characterization and application of acridine-9-N-acetyl-N-hydroxysuccinimide as a pre-column derivatization agent for fluorimetric detection of amino acids in liquid chromatography
AUTHOR(S): You, Jinmao; Lao, Wenjian; You, Jing; Wang, Guojun
CORPORATE SOURCE: Lanzhou Inst. Chem. Phys., Chinese Academy of Sciences, Lanchou, 730000, Peop. Rep. China
SOURCE: Analyst (Cambridge, United Kingdom) (1999), 124(12), 1755-1760
CODEN: ANALAO; ISSN: 0003-2654
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple and sensitive LC method that rapidly labels amino compds. including amino acids, using acridine-9-N-acetyl-N-hydroxysuccinimide (AAHS) which was synthesized by the reaction of acridine-9-N-acetic acid with benzenedisulfonyl-N-hydroxysuccinimide, was developed. A mixture of amines is treated with AAHS in the presence of triethylamine in non-aqueous acetonitrile or in 0.2 mol l-1 borate buffer at pH 8.0-9.0 in 40% volume/volume acetonitrile solution to give quant. yields of amides. The emission maximum for the derivatized amines is 435 nm (λex = 404 nm). The labeled derivs. are very stable; no significant decomposition is observed after heating in 50% acetonitrile at 40° for 24 h. Studies on the derivatization conditions indicate that amines or amino acids react very rapidly with AAHS under the proposed conditions. The method, in conjunction with a multi-step gradient, offers baseline resolution of common amine or amino acid derivs. on a reversed-phase C18 column. This method is more convenient and more efficient than previous methods which require prior conversion of carboxylic acids to acyl chlorides, which are unstable to moisture. The LC separation of amine or amino acid derivs. has good reproducibility. The established method is also suitable for the determination of other amine compds. in various biol. fluids.

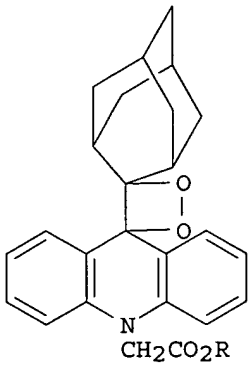
IT **150321-96-3P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(characterization and application of acridine-9-N-acetyl-N-hydroxysuccinimide as a pre-column derivatization agent for fluorimetric detection of amino acids in liquid chromatog.)

RN 150321-96-3 HCAPLUS
CN 2,5-Pyrrolidinedione, 1-[[(9-oxo-10(9H)-acridinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:106528 HCAPLUS
DOCUMENT NUMBER: 126:212075
TITLE: Synthesis and chemiluminescent property of the novel 1,2-dioxetanes containing an acridane-10-acetate moiety as the luminophor and trigger unit
AUTHOR(S): Imanishi, Takeshi; Ueda, Yohko; Tainaka, Ryoh; Miyashita, Kazuyuki; Hoshino, Nobuhiro
CORPORATE SOURCE: Faculty Pharmaceutical Sciences, Osaka Univ., Suita, 565, Japan
SOURCE: Tetrahedron Letters (1997), 38(5), 841-844
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Novel dioxetane derivs. I [R = Et, CH2CCl3, (un)substituted Ph] with an acridane-10-acetate moiety were prepared and tested as potential

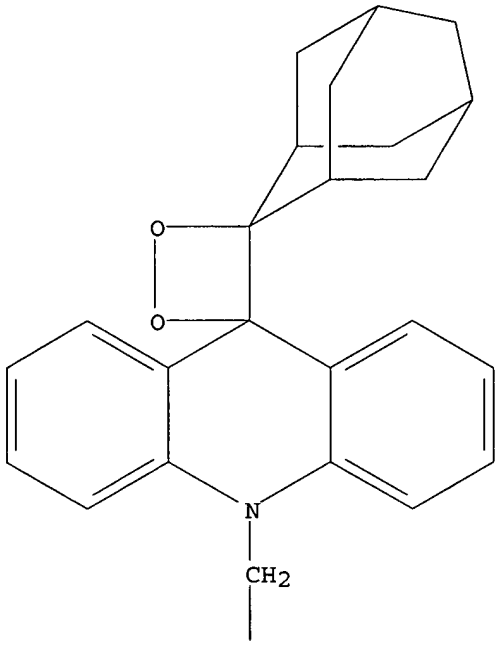
chemiluminescent probes. The 10-acetate was found to play an important role both in stabilization and in base-mediated smooth degradation of the dioxetane ring.

IT **178312-97-5P 188002-48-4P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(preparation, thermal stability, and chemiluminescence of 1,2-dioxetanes containing an acridane acetate moiety)

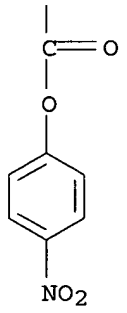
RN 178312-97-5 HCAPLUS

CN Dispiro[acridine-9(10H),3'-[1,2]dioxetane-4',2''-tricyclo[3.3.1.13,7]decane]-10-acetic acid, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



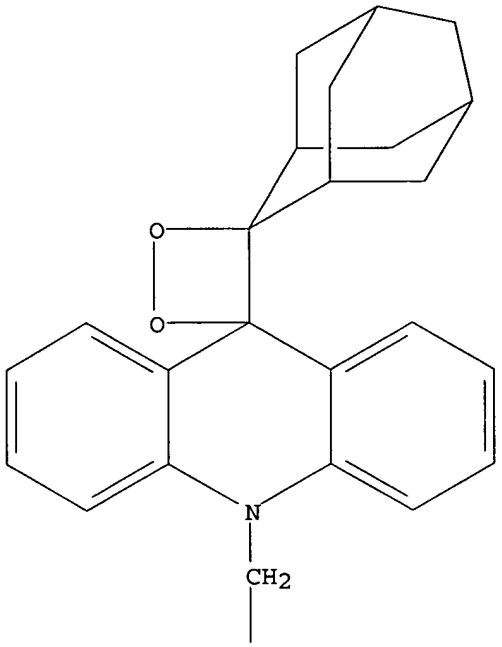
PAGE 2-A



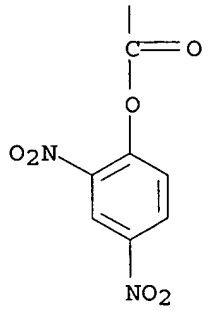
RN 188002-48-4 HCAPLUS

CN Dispiro[acridine-9(10H),3'-[1,2]dioxetane-4',2''-tricyclo[3.3.1.13,7]decane]-10-acetic acid, 2,4-dinitrophenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



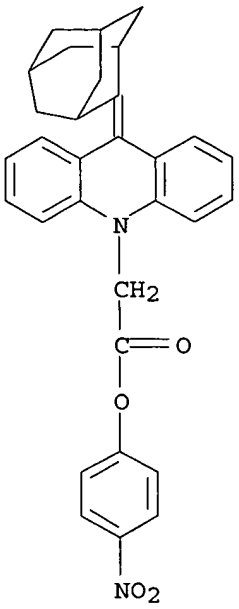
PAGE 2-A



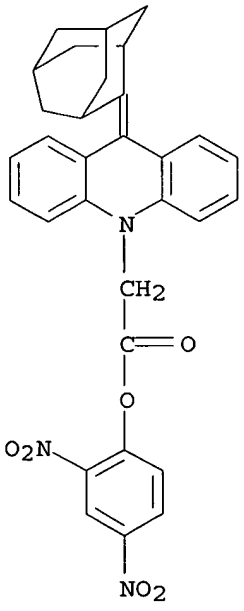
IT **178313-00-3P 188002-39-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, thermal stability, and chemiluminescence of 1,2-dioxetanes containing an acridane acetate moiety)

RN 178313-00-3 HCAPLUS

CN 10(9H)-Acridineacetic acid, 9-tricyclo[3.3.1.13,7]decylidene-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



RN 188002-39-3 HCAPLUS
CN 10(9H)-Acridineacetic acid, 9-tricyclo[3.3.1.13,7]decylidene-, 2,4-dinitrophenyl ester (9CI) (CA INDEX NAME)



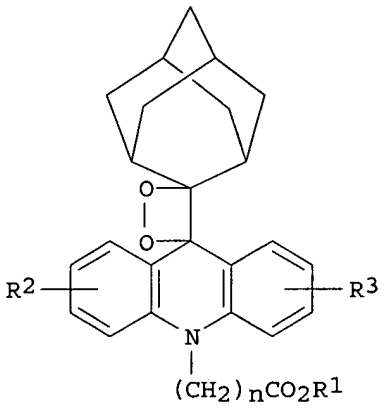
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:401584 HCAPLUS
DOCUMENT NUMBER: 125:58346

TITLE: Preparation of acridine derivatives as chemiluminescent compounds
INVENTOR(S): Imanishi, Takeshi; Hoshino, Nobuhiro; Shimamoto, Kazutoshi
PATENT ASSIGNEE(S): Iatron Lab., Japan; Mitsubishi Chemical Yatron Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08092254	A2	19960409	JP 1994-254730	19940923
JP 3551984	B2	20040811		
PRIORITY APPLN. INFO.:			JP 1994-254730	19940923

OTHER SOURCE(S): MARPAT 125:58346
GI

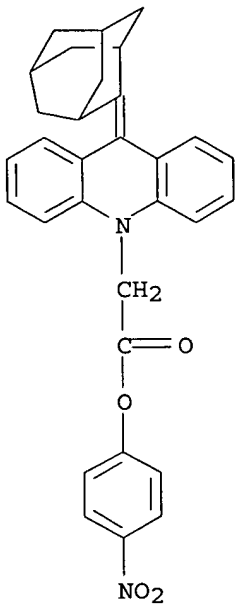


I

AB The title compds. I [n = 1 - 3; R1 = H, alkyl, etc.; R2, R3 = H, nitro, etc.] are prepared I [R2 = R3 = H; n = 1; R1 = 4-nitrophenyl] (II) (preparation given) showed chemiluminescence. II showed good storage stability.

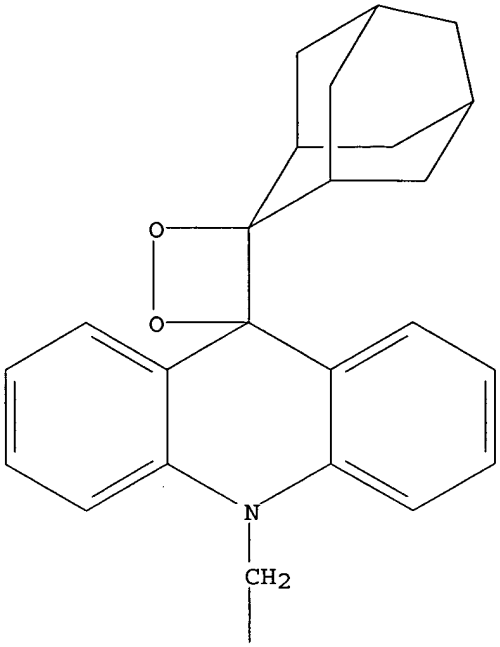
IT **178313-00-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acridine derivs. as chemiluminescent compds.)

RN 178313-00-3 HCAPLUS
CN 10(9H)-Acridineacetic acid, 9-tricyclo[3.3.1.13,7]decylidene-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

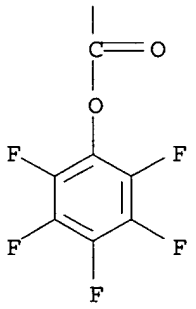


IT **178312-96-4P 178312-97-5P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acridine derivs. as chemiluminescent compds.)
RN 178312-96-4 HCAPLUS
CN Dispiro[acridine-9(10H),3'-[1,2]dioxetane-4',2''-tricyclo[3.3.1.13,7]decane]-10-acetic acid, pentafluorophenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

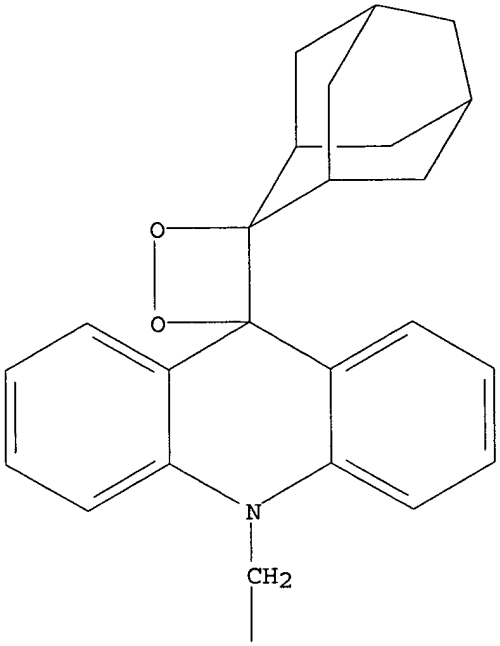


PAGE 2-A



RN 178312-97-5 HCAPLUS
CN Dispiro[acridine-9(10H),3'-[1,2]dioxetane-4',2''-tricyclo[3.3.1.13,7]decane]-10-acetic acid, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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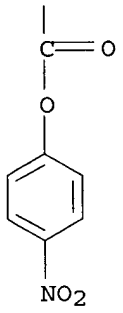

L11 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:171871 HCAPLUS
DOCUMENT NUMBER: 124:225820
TITLE: Preparation of derivatized 10,10'-substituted-9,9'-bisacridine luminescent molecules and signal solutions
INVENTOR(S): Katsilometes, George W.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9600392	A1	19960104	WO 1995-US7966	19950622
W: CN, JP, KR				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 766825	A1	19970409	EP 1995-924671	19950622
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1155931	A	19970730	CN 1995-194681	19950622
JP 10502346	T2	19980303	JP 1995-503340	19950622
US 5866335	A	19990202	US 1996-767288	19961216
HK 1001416	A1	20050826	HK 1998-100291	19980114
PRIORITY APPLN. INFO.:			US 1994-265481 A	19940624
			WO 1995-US7966 W	19950622

AB The synthesis of 10,10'-substituted-9,9'-bisacridine mols. and their derivs. is disclosed. These mols. catalyze the production of light by chemiluminescence in the presence of a signal solution having at a pH from about 10.0 to about 14.0, at a concentration effective for producing a chemiluminescent signal, a chelating agent, a sulfoxide, a reducing sugar, and oxidant or combination of oxidants, an alc. and aqueous sodium tetraborate. These 10,10'-substituted-9,9'-biacridines are used alone or attached to haptens or macromols. and are utilized as labels in the preparation of chemiluminescent, homogeneous or heterogeneous assays. They are also used in conjunction with other chemiluminescent label mols. to produce multiple analyte chemiluminescent assays. An assay demonstrating the linearity of the signal with increasing dilns. of an anti-TSH-10,10'-para-toluo-9,9'-bisacridine conjugate is described.

IT **174569-85-8**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(preparation of bisacridine luminescent derivs. and signal solns.)

RN 174569-85-8 HCAPLUS

CN 9,9'-Biacridinium, 10,10-bis[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-, dinitrate (9CI) (CA INDEX NAME)

CM 1

CRN 174569-84-7
CMF C38 H28 N4 O8

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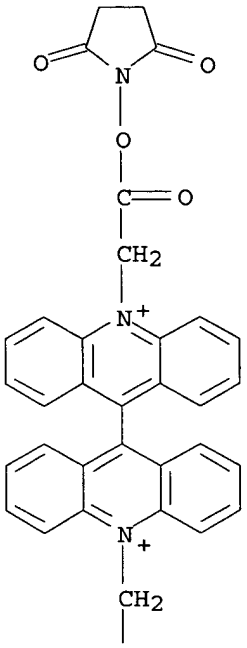
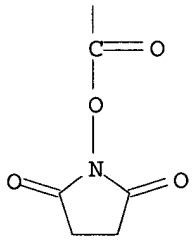
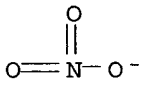


PAGE 2-A



CM 2

CRN 14797-55-8
CMF N O3



L11 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:599848 HCAPLUS
DOCUMENT NUMBER: 123:74302
TITLE: Netropsin and spermine conjugates of a water-soluble

quinocarcin analog: Analysis of sequence-specific DNA interactions

AUTHOR(S): Flanagan, Mark E.; Rollins, Samuel B.; Williams, Robert M.

CORPORATE SOURCE: Department Chemistry, Colorado State University, Ft. Collins, CO, 80523, USA

SOURCE: Chemistry & Biology (1995), 2(3), 147-56
CODEN: CBOLE2; ISSN: 1074-5521

DOCUMENT TYPE: Journal

LANGUAGE: English

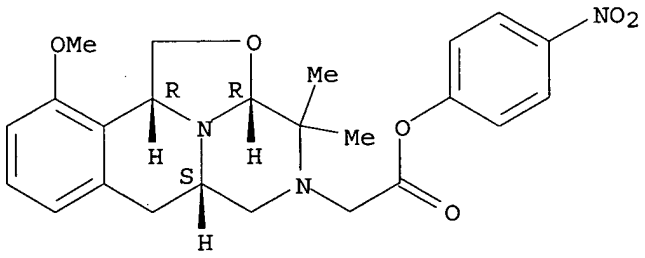
AB Quinocarcin is the simplest of the bioxalmycin/naphthyridinomycin/tetrazomine/saframycin class of antitumor antibiotics, which damage DNA in a process that is inhibited by superoxide dismutase (SOD). The oxazolidine moiety of this class of antitumor antibiotics undergoes a redox self-disproportionation reaction of the Cannizzaro type. The reaction is proposed to proceed via an intermediate carbon-centered radical, which then reduces mol. oxygen to give superoxide. We set out to determine whether the DNA-cleavage properties of these antitumor antibiotics could be retained in less complex analogs of quinocarcin. A totally synthetic, water-soluble analog of quinocarcin has been prepared This analog produced superoxide, but had considerably reduced ability to cleave supercoiled circular DNA compared to quinocarcin or tetrazomine. When conjugated to the DNA-binding mol. spermine, however, it cleaved DNA as effectively as quinocarcin at less than 1/10 the concentration A conjugate with netropsin displayed selective cleavage around the sequence 5'-d(ATTT)-3'. Mol. modeling of the interaction between the conjugate and DNA, together with the pattern of cleavage, indicates that a non-diffusable oxidant is involved in sequence-selective DNA cleavage. The spermine conjugate displayed weak antimicrobial activity. Knowledge of the stereoelectronic requirements for superoxide production by quinocarcin has allowed us to design a structurally less complex analog which has many of the same phys. properties, including water solubility, the ability to produce superoxide and the ability to cleave DNA. Covalently attaching known DNA-binding mols. to this analog gave a compound that produced sequence-specific DNA damage. Our results suggest that a mechanism other than superoxide production can mediate DNA damage by the netropsin conjugate.

IT **165253-50-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of netropsin and spermine conjugates of a water-soluble quinocarcin analog and anal. of sequence-specific DNA damage)

RN 165253-50-9 HCAPLUS

CN 2-Oxa-4,10c-diazaaceanthrylene-4(1H)-acetic acid, 2a,3,5,5a,6,10b-hexahydro-10-methoxy-3,3-dimethyl-, 4-nitrophenyl ester, (2aR,5aS,10bR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:630757 HCAPLUS
DOCUMENT NUMBER: 121:230757
TITLE: Preparation of quinolizinoxanthene derivatives and xanthene derivatives as fluorescence labeling agents
INVENTOR(S): Shiga, Masanobu
PATENT ASSIGNEE(S): Dojin Kagaku Kenkyusho Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06157504	A2	19940603	JP 1992-54478	19920128
PRIORITY APPLN. INFO.:			JP 1992-54478	19920128
OTHER SOURCE(S):	MARPAT 121:230757			

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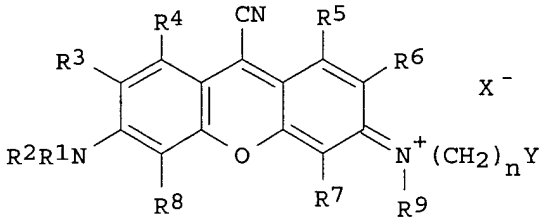
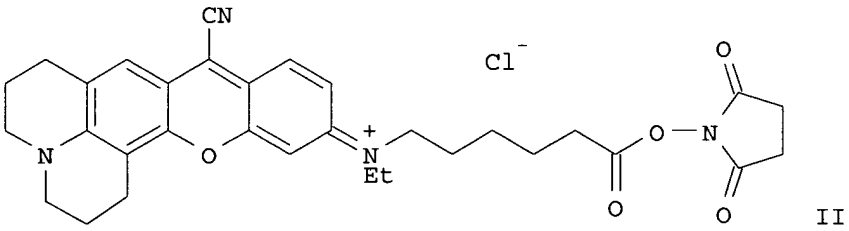
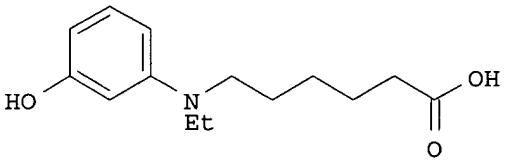


I



II

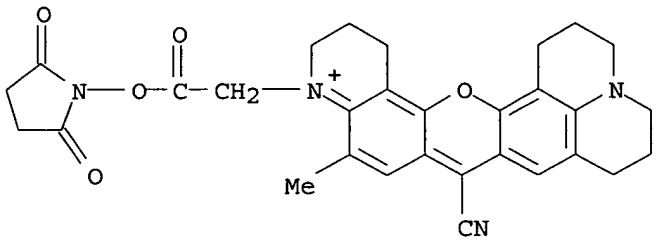


III

AB The title compds. I [R1, R2, R9 = alkyl; or R1R8, R2R3, R9R6, or R9R7 = ring; R3,R4,R6 - R8 = H, alkyl; n = 1 - 10; Y = carboxy, etc.; X = halo] are prepared Quinolizinoxanthene II was prepared in a multiple step process starting with aminophenol derivative III. The anal. of amino acids was demonstrated using a fluorescence labeling agent of this invention.

IT **158358-63-5P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(preparation of quinolizinoxanthene derivs. and xanthene derivs. as

fluorescence labeling agents)
RN 158358-63-5 HCAPLUS
CN 1H,9H,13H-Pyrido[3',2':5,6]xantheno[2,3,4-ij]quinolizinium, 7-cyano-4-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-2,3,10,11,14,15-hexahydro-5-methyl-, chloride (9CI) (CA INDEX NAME)

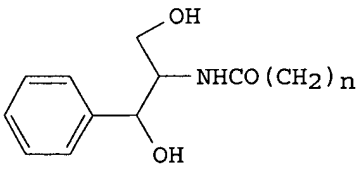


● Cl⁻

L11 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:435864 HCAPLUS
DOCUMENT NUMBER: 121:35864
TITLE: Fluorescent chloramphenicol derivatives for determination of chloramphenicol acetyltransferase activity
INVENTOR(S): Haughland, Richard P.; Kang, Hee C.; Young, Steven L.; Melner, Michael H.
PATENT ASSIGNEE(S): Molecular Probes, Inc., USA
SOURCE: U.S., 13 pp. Cont. of U.S. Ser. No. 321,494, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5262545	A	19931116	US 1991-722352	19910618
US 5364764	A	19941115	US 1992-994992	19921221
PRIORITY APPLN. INFO.:			US 1989-321494 B1	19890309
			US 1991-722352 A3	19910618

OTHER SOURCE(S): MARPAT 121:35864
GI



I

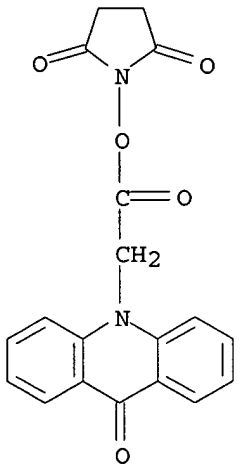
AB Fluorescent compds. useful in the determination of chloramphenicol

acetyltransferase (CAT) enzyme activity are described. The compds. BASE-Ns-*X are fluorescent derivs. related in structure to chloramphenicol comprising a base (I), substituted at one to five aromatic ring positions by substituents, which may be the same or different, that are alkyl, hydroxy, alkoxy, aryl, halo, nitro, amino, alkylamido, or arylamido, and 0 < n < 6; and a fluorescent moiety *X (nonreduced tricyclic difluoroboradiazaindacene fluorophore) linked to the terminal CH2 of BASE through a linker Ns (e.g., NH*X, NHCOCH2*X). The substrate compds. are acylated in the presence of CAT to produce fluorescent mono- and diacylated products, which are then phys. separated from the reaction mixture and quantitated by means of their fluorescence and/or absorbance. Fluorescent mols. conjugated to chloramphenicol include derivs. of fluorescein, rhodamine, coumarin, dimethylaminonaphthalenesulfonic acid (dansyl), pyrene, anthracene, nitrobenzoxadiazole (NBD), acridine and dipyrromethene boron difluoride.

IT **150321-96-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorescent chloramphenicol derivs. for determination of chloramphenicol acetyltransferase activity)

RN 150321-96-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(9-oxo-10(9H)-acridinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



L11 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:101282 HCAPLUS
DOCUMENT NUMBER: 120:101282
TITLE: Fluorescent energy transfer immunoassay
INVENTOR(S): Lakowicz, Joseph; Maliwal, Badri; Thompson, Richard; Ozinskas, Alvydas
PATENT ASSIGNEE(S): University of Maryland, USA
SOURCE: Eur. Pat. Appl., 26 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

EP 552108	A2	19930721	EP 1993-400091	19930115
EP 552108	A3	19930922		
R: DE, FR, GB, IT				
CA 2087413	AA	19930718	CA 1993-2087413	19930115
JP 06066802	A2	19940311	JP 1993-6057	19930118
JP 3325939	B2	20020917		
US 5631169	A	19970520	US 1994-183238	19940119

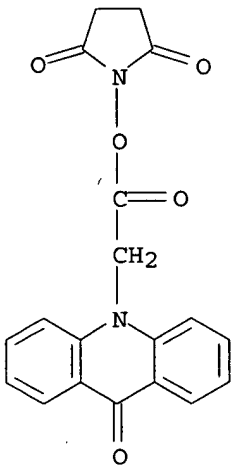
PRIORITY APPLN. INFO.: US 1992-822233 A 19920117

AB A photoluminometric immunoassay comprises reacting 2 immunoreactants, 1 labeled with a photoluminescent energy transfer donor capable of photoluminescence and the other labeled with a photoluminescent energy transfer acceptor complementary to the donor; exciting the sample with radiation; and calculating the apparent luminescence lifetime to determine the presence of a reaction product. Studies were done using goat anti-mouse IgG labeled with the donor dichlorotriazinylaminofluorescein and mouse IgG labeled with the acceptor tetramethylrhodamine isothiocyanate.

IT **150321-96-3D**, conjugates with immunoreactant
RL: ANST (Analytical study)
(in photoluminometric immunoassay)

RN 150321-96-3 HCAPLUS

CN 2,5-Pyrrolidinedione, 1-[[(9-oxo-10(9H)-acridinyl)acetyl]oxy]- (9CI) (CA INDEX NAME)



L11 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER:	1991:535937 HCAPLUS
DOCUMENT NUMBER:	115:135937
TITLE:	Preparation of N-[[(alkylideneimino)oxycarbonyl]alkyl]-1,8-naphthalenedicarboximides and analogs as herbicide safeners
INVENTOR(S):	Saupe, Thomas; Meyer, Norbert; Plath, Peter; Schirmer, Ulrich; Wuerzer, Bruno; Westphalen, Karl Otto; Patsch, Manfred; Pfister, Juergen
PATENT ASSIGNEE(S):	BASF A.-G., Germany
SOURCE:	Eur. Pat. Appl., 45 pp. CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 430004	A2	19910605	EP 1990-122030		19901117
EP 430004	A3	19911218			
R: AT, CH, DE, ES, FR, GB, IT, LI, NL, SE					
DE 3939379	A1	19910606	DE 1989-3939379		19891129
DE 4021654	A1	19920109	DE 1990-4021654		19900707
CA 2030129	AA	19910530	CA 1990-2030129		19901116
US 5076831	A	19911231	US 1990-615865		19901120
JP 03190861	A2	19910820	JP 1990-323392		19901128
PRIORITY APPLN. INFO.:			DE 1989-3939379	A	19891129
			DE 1990-4021654	A	19900707

OTHER SOURCE(S): MARPAT 115:135937
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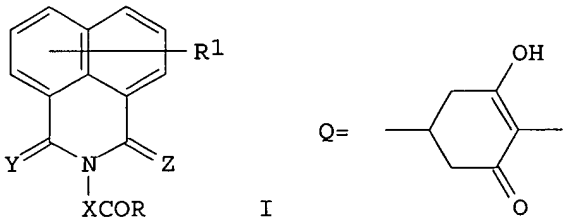
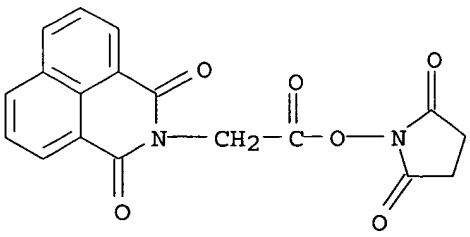


AB The title compds. [I; R = ON:CR5R6; R1 = 1-4 substituents which may be the same or different selected from H, halo, cyano, (halo)alkyl, etc.; R5 = H, cyano, alkyl, alkenyl, etc.; R6 = H, cyano, (halo)alkyl, alkoxy, etc.; X = (un)substituted alkylene; Y, Z = O, S] were prepared as safeners for 2-[(hetero)aryloxyphenoxy]acetate and -propionate or alkoximinomethylenecycylohexenone herbicides. Thus, I (R1 = H, X = CH2, Y = Z = O) (II); R = Cl) (preparation given) was condensed with Me2C:NOH to give II (R = ON:CMe2). II [R = ON:CR5R6; R5R6 = (CH2)3CH:C(OEt)] reduced damage to wheat of 0.03 kg/ha of the herbicide EtSCHMEH2Z1C(:NOEt)Pr (Z1 = hydroxycyclohexenonylene group Q) from 70 to 10% (with 95% control of annual ryegrass) at 0.125 kg/ha.

IT **135980-49-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as herbicide safener)

RN 135980-49-3 HCAPLUS

CN 1H-Benz[de]isoquinoline-1,3(2H)-dione, 2-[2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]- (9CI) (CA INDEX NAME)



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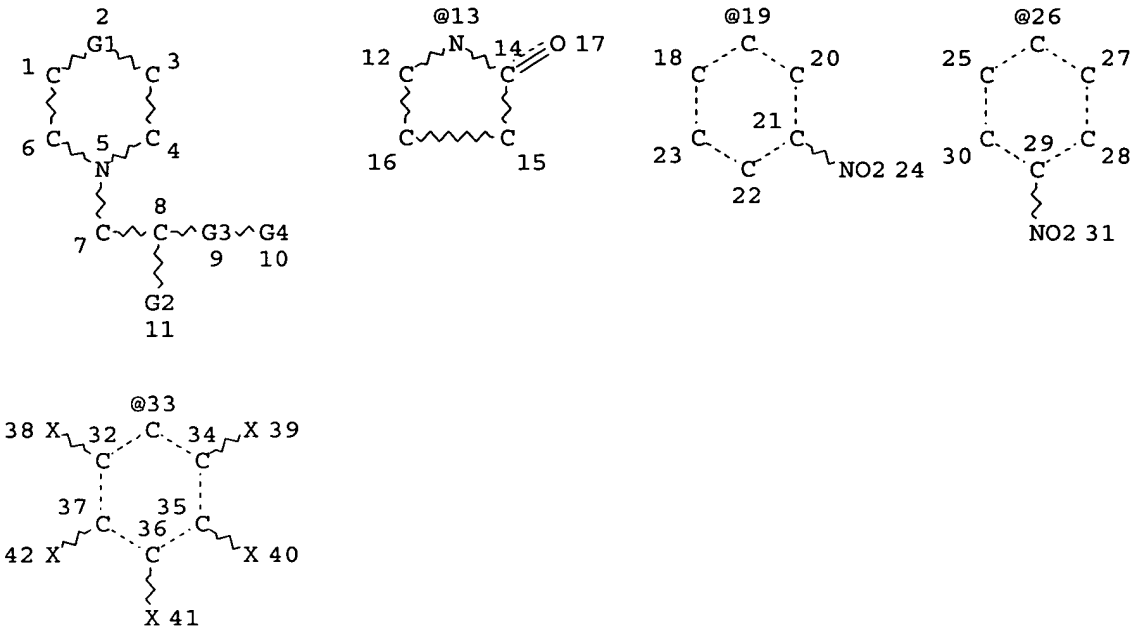

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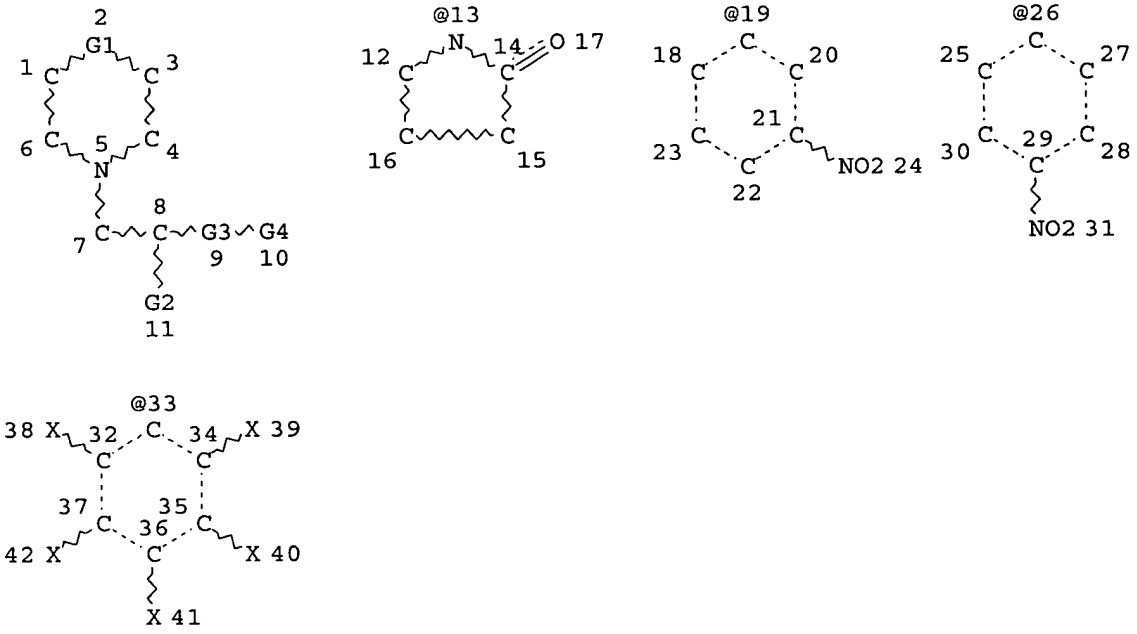
VAR G3=O/S
VAR G4=13/19/26/33
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
L5 82 SEA FILE=REGISTRY SSS FUL L1
L6 STR



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NUMBER OF NODES IS 42

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L8 29 SEA FILE=HCAPLUS ABB=ON PLU=ON L7
L9 36 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L7
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L11 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT L8
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L13 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:19284 HCAPLUS
DOCUMENT NUMBER: 142:257250
TITLE: Multiplexed protein quantitation in Saccharomyces cerevisiae using amine-reactive isobaric tagging reagents
AUTHOR(S): Ross, Philip L.; Huang, Yulin N.; Marchese, Jason N.; Williamson, Brian; Parker, Kenneth; Hattan, Stephen; Khainovski, Nikita; Pillai, Sasi; Dey, Subhakar; Daniels, Scott; Purkayastha, Subhasish; Juhasz, Peter; Martin, Stephen; **Bartlet-Jones, Michael**; He,

Feng; Jacobson, Allan; Pappin, Darryl J.
CORPORATE SOURCE: Applied Biosystems, Framingham, MA, 01701, USA
SOURCE: Molecular and Cellular Proteomics (2004), 3(12), 1154-1169
CODEN: MCPOBS; ISSN: 1535-9476
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We describe here a multiplexed protein quantitation strategy that provides relative and absolute measurements of proteins in complex mixts. At the core of this methodol. is a multiplexed set of isobaric reagents that yield amine-derivatized peptides. The derivatized peptides are indistinguishable in MS, but exhibit intense low-mass MS/MS signature ions that support quantitation. In this study, we have examined the global protein expression of a wild-type yeast strain and the isogenic upf1Δ and xrn1Δ mutant strains that are defective in the nonsense-mediated mRNA decay and the general 5' to 3' decay pathways, resp. We also demonstrate the use of 4-fold multiplexing to enable relative protein measurements simultaneously with determination of absolute levels of a target protein using synthetic isobaric peptide stds. We find that inactivation of Upf1p and Xrn1p causes common as well as unique effects on protein expression.

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:442251 HCAPLUS
DOCUMENT NUMBER: 141:238084
TITLE: Urinary N2-(2'-deoxyguanosin-8-yl)PhIP as a biomarker for PhIP exposure
AUTHOR(S): Fang, Min; Edwards, Robert J.; **Bartlet-Jones, Michael**; Taylor, Graham W.; Murray, Stephen; Boobis, Alan R.
CORPORATE SOURCE: Section of Experimental Medicine and Toxicology, Imperial Coll. London, London, W12 0NN, UK
SOURCE: Carcinogenesis (2004), 25(6), 1053-1062
CODEN: CRNGDP; ISSN: 0143-3334
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The food-derived, heterocyclic aromatic amine 2-amino-1-methyl-6-phenylimidazo[4,5-b]pyridine (PhIP) is genotoxic and is carcinogenic in exptl. animals. Studies on the role of PhIP in human diet-related cancer would be aided considerably by the availability of a readily applicable biomarker of the internal dose of the ultimate genotoxic species. PhIP has been shown to adduct primarily at C-8 of deoxyguanosine in DNA and so the DNA repair product N2-(2'-deoxyguanosin-8-yl)PhIP is a potential biomarker of DNA adduction and repair after exposure to PhIP. An assay for N2-(2'-deoxyguanosin-8-yl)PhIP in urine has been developed based on liquid chromatog. mass spectrometry, using a deuterated analog of the nucleoside as an internal standard and an antibody-mediated extraction procedure.

Polyclonal antibodies were raised against the PhIP-nucleotide, PhIP-nucleoside and PhIP-guanine base adducts conjugated to keyhole limpet hemocyanin. Following their evaluation, the immobilized PhIP nucleotide antibody was used for the extraction of N2-(2'-deoxyguanosin-8-yl)PhIP from urine. The limit of detection of the assay was 125 pg and the limit of quantification 200 pg for a 50 mL human urine sample. Following oral

administration of PhIP (20 mg/kg body wt/day) to rats for 6 days, N2-(2'-deoxyguanosin-8-yl) PhIP was readily detected in the urine, reaching steady state over 3 days. This is the first direct demonstration of the urinary elimination of this adduct following exposure to parent amine. The half-life of the adduct with DNA was estimated to be .apprx.20 h. The total amount of PhIP recovered in the urine as adduct was <0.5 + 10-3% of the dose administered. Levels of the PhIP adduct in urine collections from human subjects ingesting the amine (4.9 μg) in cooked meat were below the limits of detection, indicating that humans are exposed to a bioactive dose of <3 + 10-4 of that associated with a non-carcinogenic level in rats.

REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:868721 HCAPLUS
DOCUMENT NUMBER: 136:31639
TITLE: Method of stimulating non-homologous end-joining (NHEJ) of DNA in the presence of inositol phosphate and drug screening systems and assays for compounds that modulate NHEJ
INVENTOR(S): West, Steve Craig; Hanakahi, Leslyn Ann Akemi; **Bartlet-Jones, Michael**
PATENT ASSIGNEE(S): Imperial Cancer Research Technology Limited, UK
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090404	A1	20011129	WO 2001-GB2180	20010518
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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EP 1283903	A1	20030219	EP 2001-929850	20010518
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004500849	T2	20040115	JP 2001-586599	20010518
US 2004029130	A1	20040212	US 2003-296014	20030612
PRIORITY APPLN. INFO.:			GB 2000-12179 A	20000520
			US 2000-221226P P	20000725
			US 2001-268367P P	20010214
			WO 2001-GB2180 W	20010518

AB A method of stimulating non-homologous end-joining (NHEJ) of DNA the method comprising performing NHEJ of DNA in the presence of inositol hexakisphosphate (IP6) or other stimulatory inositol phosphate. An assay of a protein kinase wherein the assay comprises inositol hexakisphosphate (IP6) or other stimulatory inositol phosphate. The invention also provides screening assays for compds. which may modulate NHEJ and which may be therapeutically useful; and screening assays for compds. which may

modulate DNA-PK and related protein kinases and which may be therapeutically useful. Methods of modulating NHEJ and protein kinases are also disclosed. Compns. and kits that may be useful in performing the assays and methods of the invention are also claimed.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:690240 HCAPLUS
DOCUMENT NUMBER: 133:330378
TITLE: Binding of inositol phosphate to DNA-PK and stimulation of double-strand break repair
AUTHOR(S): Hanakahi, Les A.; **Bartlet-Jones, Michael**; Chappell, Claire; Pappin, Darryl; West, Stephen C.
CORPORATE SOURCE: Imperial Cancer Research Fund Clare Hall Laboratories, South Mimms, EN6 3LD, UK
SOURCE: Cell (Cambridge, Massachusetts) (2000), 102(6), 721-729
CODEN: CELLB5; ISSN: 0092-8674
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In mammalian cells, double-strand breaks in DNA can be repaired by nonhomologous end-joining (NHEJ), a process dependent upon Ku70/80, DNA-PKCS, XRCC4, and DNA ligase IV. Starting with HeLa cell-free exts., which promote NHEJ in a reaction dependent upon all of these proteins, we have purified a novel factor that stimulates DNA end-joining in vitro. Using a combination of phosphorus NMR, mass spectroscopy, and strong anion exchange chromatog., we identify this factor as inositol hexakisphosphate (IP6). Purified IP6 is bound by DNA-PK and specifically stimulates DNA-PK-dependent end-joining in vitro. The involvement of inositol phosphate in DNA-PK-dependent NHEJ is of particular interest since the catalytic domain of DNA-PKCS is similar to that found in the phosphatidylinositol 3 (PI 3)-kinase family.

L13 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:293327 HCAPLUS
DOCUMENT NUMBER: 131:128721
TITLE: Dual specificity antibodies using a double-stranded oligonucleotide bridge
AUTHOR(S): Chaudri, Zahida N.; **Bartlet-Jones, Michael**; Panayotou, George; Klonisch, Thomas; Roitt, Ivan M.; Lund, Torben; Delves, Peter J.
CORPORATE SOURCE: Department of ImmunologyThe Windeyer Institute for Medical Sciences, University College London, London, W1P 6DB, UK
SOURCE: FEBS Letters (1999), 450(1,2), 23-26
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The covalent conjugation of oligonucleotides to antibody Fab' fragments was optimized by using oligonucleotides modified with a hexaethylene linker arm bearing three amino groups. One oligonucleotide was coupled to antibody of one specificity and a complementary oligonucleotide to antibody of a second specificity. The antibodies were then allowed to hybridize by base pairing of the complementary nucleotide sequences and the generation of bispecific antibody was analyzed on SDS-PAGE and confirmed using BIAcore anal. The strategy of complementary oligonucleotide-linked bispecific mols. is not limited to antibodies but

is applicable to linking any two mols. of different characteristics.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:811809 HCAPLUS
DOCUMENT NUMBER: 128:154377
TITLE: Peptide sequencing of charged derivatives by postsource decay MALDI mass spectrometry
AUTHOR(S): Spengler, Bernhard; Luetzenkirchen, Frank; Metzger, Sabine; Chaurand, Pierre; Kaufmann, Raimund; Jeffery, William; **Bartlet-Jones, Michael**; Pappin, Darryl J. C.
CORPORATE SOURCE: P.O. Box 101007, Institute of Laser Medicine and Center for Biological and Medical Research, University of Dusseldorf, Dsseldorf, D-40001, Germany
SOURCE: International Journal of Mass Spectrometry and Ion Processes (1997), 169/170, 127-140
CODEN: IJMPDN; ISSN: 0168-1176
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Derivatization procedures for peptides are described that can be performed with sub-picomolar amts. of sample and that are able to direct the formation of fragment ions in Postsource Decay (PSD) MALDI mass spectrometry. Location of a fixed charge (a quaternary ammonium ion) at the N-terminus of a peptide and modification of internal arginine residues (deletion of strong basicity) leads to a full controllability of fragment ion formation resulting in mostly complete series of N-terminal fragment ions. The method appears to be favorably applicable to sequence anal. of unknown peptides, since in most cases the amino acid sequence can directly be read from the spectrum.
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:236716 HCAPLUS
DOCUMENT NUMBER: 124:311580
TITLE: Chemistry, mass spectrometry and peptide-mass databases: Evolution of methods for the rapid identification and mapping of cellular proteins
AUTHOR(S): Pappin, D. J. C.; Rahman, D.; Hansen, H. F.; **Bartlet-Jones, M.**; Jeffery, W.; Bleasby, A. J.
CORPORATE SOURCE: Imperial Cancer Research Fund, London, WC2A 3PX, UK
SOURCE: Mass Spectrometry in the Biological Sciences (1996), 135-50. Editor(s): Burlingame, A. L.; Carr, Steven A. Humana: Totowa, N. J.
CODEN: 62PNAY
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Chemical, mass spectrometry, and peptide-mass databases, and methods for the identification of proteins are described,.

L13 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:159505 HCAPLUS
DOCUMENT NUMBER: 124:255185
TITLE: Synthesis, evaluation and application of a panel of novel reagents for stepwise degradation of polypeptides
AUTHOR(S): Bures, Edward J.; Nika, Heinz; Chow, David T.; Hess,

Daniel; Morrison, Hamish D.; **Bartlet-Jones, Michael**; Pappin, Darryl J. C.; Aebersold, Ruedi
CORPORATE SOURCE: Biomedical Research Centre, University British Columbia, Vancouver, Can.
SOURCE: Methods in Protein Structure Analysis, [Proceedings of the International Conference on Methods in Protein Structure Analysis], 10th, Snowbird, Utah, Sept. 8-13, 1994 (1995), Meeting Date 1994, 57-68. Editor(s): Atassi, M. Zouhair; Appella, Ettore. Plenum: New York, N. Y.
CODEN: 62LPAK
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The authors synthesized and evaluated a panel of novel protein sequencing reagents designed to yield amino acid derivs. detectable at the low-femtomole level by electrospray-ionization mass spectrometry (ESI-MS). Protein degradation with these reagents is based on the Ph isothiocyanate functionality introduced by Edman. The chemistries were easily adapted to automated stepwise degradation Through a systematic process, the authors arrived at a new reagent, 4-(3-pyridinylmethylaminocarboxypropyl)phenyl isothiocyanate (PITC 311), that permits a sequencing approach that incorporates ESI-MS detection. By using this approach, they showed that PITC 311 is compatible with femtomole level peptide sequencing. Also mass information provided by ESI-MS detection enhances the confidence level in data interpretation. Mass information available by ESI-MS anal. of 311 PTHs assists in characterization of modified and unnatural amino acid residues. The authors aim to optimize automated sequencing cycles for high sensitivity protein sequencing, and to develop a methodol. to apply PITC 311 for high-sensitivity absorptive sequencing, and to create rapid sequencing protocols.

L13 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:604181 HCAPLUS
DOCUMENT NUMBER: 123:78926
TITLE: The use of a volatile N-terminal degradation reagent for rapid, high-sensitivity sequence analysis of peptides by generation of sequence ladders
AUTHOR(S): **Bartlet-Jones, M.**; Jeffery, W. A.; Hansen, H. F.; Pappin, D. J. C.
CORPORATE SOURCE: Protein Sequencing Lab., Imperial Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Tech. Protein Chem. VI, [Pap. Symp. Protein Soc.], 8th (1995), Meeting Date 1994, 3-11. Editor(s): Crabb, John W. Academic: San Diego, Calif.
CODEN: 61MDAG
DOCUMENT TYPE: Conference
LANGUAGE: English

AB The aim of this work was to explore sequencing strategies capable of rapid anal. of proteins, possibly recovered from 2-D electrophoresis gels. For this purpose, the chemical needed to be adaptable to multiple samples and sensitive enough to work in the femtomole range. The described trifluoroethyl isothiocyanate chemical is showing early signs of meeting these criteria. The demonstration, on a low-picomolar scale, that a phosphorylated tyrosine residue could be directly identified make this a potentially powerful tool for the identification of this and other sites of posttranslational modification. The inherent simplicity of the process should also allow for easy automation to permit rapid processing of samples in parallel.

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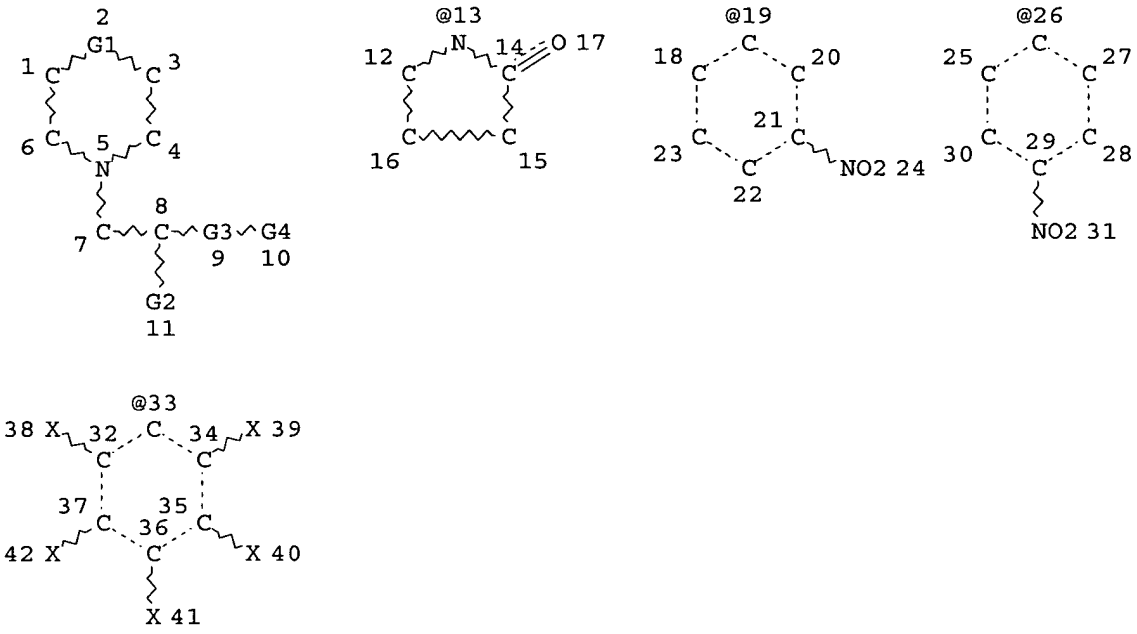

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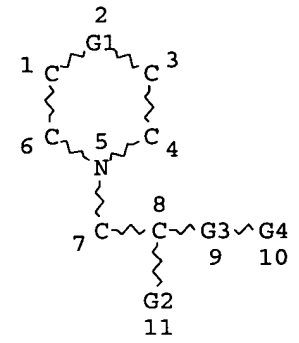

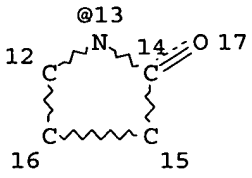

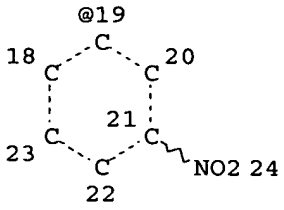

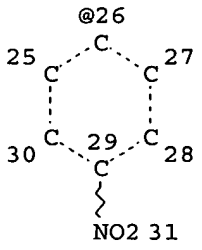

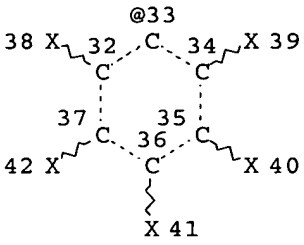

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GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE

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L9 36 SEA FILE=REGISTRY ABB=ON PLU=ON L5 NOT L7
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L11 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 NOT L8
L12 103 SEA FILE=HCAPLUS ABB=ON PLU=ON ("PAPPIN D"/AU OR "PAPPIN D J"/AU OR "PAPPIN D J C"/AU OR "PAPPIN DARRYL"/AU OR "PAPPIN DARRYL J"/AU OR "PAPPIN DARRYL J C"/AU OR "PAPPIN DARRYL JOHN CECIL"/AU OR "PAPPIN DARYL"/AU) NOT (L8 OR L11)
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L16 ANSWER 1 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:296950 HCAPLUS
DOCUMENT NUMBER: 140:402642
TITLE: Suppression of α-Cyano-4-hydroxycinnamic Acid

Matrix Clusters and Reduction of Chemical Noise in MALDI-TOF Mass Spectrometry
AUTHOR(S): Smirnov, I. P.; Zhu, X.; Taylor, T.; Huang, Y.; Ross, P.; Papayanopoulos, I. A.; Martin, S. A.; **Pappin, D. J.**
CORPORATE SOURCE: Applied Biosystems, Framingham, MA, 01701, USA
SOURCE: Analytical Chemistry (**2004**), 76(10), 2958-2965
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Progress in high-throughput MALDI-TOFMS **anal.**, especially in proteome applications, requires development of practical and efficient procedures for the preparation of proteins and peptides in a form suitable for high acquisition rates. These methods should improve successful identification of peptides, which depends on the signal intensity and the absence of interfering signals. Contamination of MALDI samples with alkali salts results in reduced MALDI peptide sensitivity and causes matrix cluster formation (widely reported for CHCA matrix) observed as signals dominating in the range below m/z 1200 in MALDI spectra. One way to remove these background signals, especially for concns. of peptides lower than 10 fmol/μL, is to wash matrix/sample spots after peptide cocrystn. on the MALDI plate with deionized water prior to **anal.** This method takes advantage of the low water solubility of the CHCA compared to its alkali salts. We report here that the application of some ammonium salt solns., such as citrates and phosphates, instead of deionized water greatly improves the efficiency of this washing approach. Another way to reduce matrix cluster formation is to add ammonium salts as a part of the MALDI matrix. The best results were obtained with monoammonium phosphate, which successfully suppressed matrix clusters and improved sensitivity. Combining both of these approaches-the addition of ammonium salts in the CHCA matrix followed by one postcrystn. washing step with ammonium buffer-provided a substantial (.apprx.3-5-fold) improvement in the sensitivity of MALDI-MS detection compared to unwashed sample spots. This sample preparation method resulted in improved spectral quality and was essential for successful database searching for subnanomolar concns. of protein digests.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 2 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:99057 HCAPLUS
DOCUMENT NUMBER: 138:151879
TITLE: Serological and proteomic evaluation of antibody responses in the identification of tumor antigens in renal cell carcinoma
AUTHOR(S): Unwin, Richard D.; Harnden, Patricia; **Pappin, Darryl**; Rahman, Dinah; Whelan, Peter; Craven, Rachel A.; Selby, Peter J.; Banks, Rosamonde E.
CORPORATE SOURCE: Cancer Research UK Clinical Cancer Centre, St. James's University Hospital, Leeds, LS9 7TF, UK
SOURCE: Proteomics (**2003**), 3(1), 45-55
CODEN: PROTC7; ISSN: 1615-9853
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Renal cell carcinoma (RCC) is relatively resistant to conventional chemotherapy and radiotherapy. However, reports of spontaneous regression along with promising results in clin. trials suggest that immunotherapuetic strategies may be of clin. benefit. Few RCC related

antigens have been identified to date, and the tech. difficulty and time constraints of current antigen identification techniques preclude the screening of large nos. of patients. A comparatively rapid strategy has been used to identify components of tumors that elicit an antibody response in the patient - the serol. and proteomic evaluation of antibody responses (SPEAR) approach. This combines two-dimensional polyarylamide gel electrophoresis of tumor and normal kidney samples with immunoblotting using autologous patient sera and protein identification by mass spectrometry. Using the SPEAR approach to screen RCC patients for naturally occurring antitumor antibody responses, a number of candidate immunogens have been identified in patients with high-grade disease and their relative expression levels in tumor tissue compared to normal tissue have been studied. These proteins include annexins I and IV, thymidine phosphorylase (TP), carbonic anhydrase I, Mn-superoxide dismutase and major vault protein (MVP). Downstream **anal.** of the tissue expression of some of these proteins shows that MVP is up-regulated in 2/4 of RCC tumors but is also expressed in normal kidney whereas TP is up-regulated in 100% (11/11) of RCC cases examined with no or minimal expression in normal kidney, indicating a potential use as a therapeutic target.

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 3 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:933437 HCAPLUS
DOCUMENT NUMBER: 139:176070
TITLE: Peptide mass fingerprinting using MALDI-TOF mass spectrometry
AUTHOR(S): **Pappin, Darryl J. C.**
CORPORATE SOURCE: Imperial College, University of London, London, UK
SOURCE: Methods in Molecular Biology (Totowa, NJ, United States) (**2003**), 211(Protein Sequencing Protocols (2nd Edition)), 211-219
CODEN: MMBIED; ISSN: 1064-3745
PUBLISHER: Humana Press Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The protocols that permit reliable peptide maps to be obtained from subpicomole quantities of material using matrix-assisted laser-desorption ionization time-of-flight (MALDI-TOF) mass spectrometry (MS) are described. The procedures consist of staining of electroblotted proteins; enzymic digestion and elution of peptides; esterification of peptide mixts.; MS **anal.** using MALDI; and database searches.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:724627 HCAPLUS
DOCUMENT NUMBER: 136:36207
TITLE: Changes in gene expression in macrophages infected with Mycobacterium tuberculosis: a combined transcriptomic and proteomic approach
AUTHOR(S): Ragno, Silvia; Romano, Maria; Howell, Steven; **Pappin, Darryl J. C.**; Jenner, Peter J.; Colston, Michael J.
CORPORATE SOURCE: Division of Mycobacterial Research, The National Institute for Medical Research, London, NW7 1AA, UK
SOURCE: Immunology (**2001**), 104(1), 99-108
CODEN: IMMUAM; ISSN: 0019-2805
PUBLISHER: Blackwell Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English
AB We investigated the changes which occur in gene expression in the human macrophage cell line, THP1, at 1, 6 and 12 h following infection with Mycobacterium tuberculosis. The **anal.** was carried out at the transcriptome level, using microarrays consisting of 375 human genes generally thought to be involved in immunoregulation, and at the proteomic level, using two-dimensional gel electrophoresis and mass spectrometry. The **anal.** of the transcriptome using microarrays revealed that many genes were up-regulated at 6 and 12 h. Most of these genes encoded proteins involved in cell migration and homing, including the chemokines interleukin (IL)-8, osteopontin, monocyte chemotactic protein-1 (MCP-1), macrophage inflammatory protein-1α (MIP-1α), regulated on activation, normal, T-cell expressed and secreted (RANTES), MIP-1β, MIP-3α, myeloid progenitor inhibitory factor-1 (MPIF-1), pulmonary and activation regulated chemokine (PARC), growth regulated gene-β (GRO-β), GRO-γ, MCP-2, I-309, and the T helper 2 (Th2) and eosinophil-attracting chemokine, eotaxin. Other genes involved in cell migration which were up-regulated included the matrix metalloproteinase MMP-9, vascular endothelial growth factor (VEGF) and its receptor Flk-1, the chemokine receptor CCR3, and the cell adhesion mols. vesicular cell adhesion mol.-1 (VCAM-1) and integrin α3. In addition to the chemokine response, genes encoding the proinflammatory cytokines IL-1β (showing a 433-fold induction), IL-2 and tumor necrosis factor-α (TNF-α), were also found to be induced at 6 and/or 12 h. It was more difficult to detect changes using the proteomic approach. Nevertheless, IL-1β was again shown to be strongly up-regulated. The enzyme manganese superoxide dismutase was also found to be strongly up-regulated; this enzyme was found to be macrophage-, rather than M. tuberculosis, derived. The heat-shock protein hsp27 was found to be down-regulated following infection. We also identified a mycobacterial protein, the product of the atpD gene (thought to be involved in the regulation of cytoplasmic pH) in the infected macrophage exts.
REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 5 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:269897 HCAPLUS
DOCUMENT NUMBER: 133:70658
TITLE: Hydrophobic protein that copurifies with human brain acetylcholinesterase: amino acid sequence, genomic organization, and chromosomal localization
AUTHOR(S): Navaratnam, Dhasakumar S.; Fernando, F. Shama; Priddle, John D.; Giles, Kurt; Clegg, Sheila M.; **Pappin, Darryl J.**; Craig, Ian; Smith, A. David
CORPORATE SOURCE: Department of Pharmacology, University of Oxford, Oxford, UK
SOURCE: Journal of Neurochemistry (**2000**), 74(5), 2146-2153
CODEN: JONRA9; ISSN: 0022-3042
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mechanism of attachment of acetylcholinesterase (AChE) to neuronal membranes in interneuronal synapses is poorly understood. We have isolated, sequenced, and cloned a hydrophobic protein that co-purifies with AChE from human caudate nucleus and that we propose forms a part of a complex of membrane proteins attached to this enzyme. It is a short protein of 136 amino acids and has a mol. mass of 18 kDa. The sequence contains stretches of both hydrophobic and hydrophilic amino acids and two

cysteine residues. **Anal.** of the genomic sequence reveals that the coding region is divided among five short exons. Fluorescence in situ hybridization localizes the gene to chromosome 6p21.32-p21.2. Northern blot **anal.** shows that this gene is widely expressed in the brain with an expression pattern that parallels that of AChE.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 6 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:11945 HCAPLUS
DOCUMENT NUMBER: 132:148648
TITLE: Probability-based protein identification by searching sequence databases using mass spectrometry data
AUTHOR(S): Perkins, David N.; **Pappin, Darryl J. C.**; Creasy, David M.; Cottrell, John S.
CORPORATE SOURCE: Imperial Cancer Research Fund, London, WC2A 3PX, UK
SOURCE: Electrophoresis (**1999**), 20(18), 3551-3567
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several algorithms have been described in the literature for protein identification by searching a sequence database using mass spectrometry data. In some approaches, the exptl. data are peptide mol. wts. from the digestion of a protein by an enzyme. Other approaches use tandem mass spectrometry (MS/MS) data from one or more peptides. Still others combine mass data with amino acid sequence data. We present results from a new computer program, Mascot, which integrates all three types of search. The scoring algorithm is probability based, which has a number of advantages: (i) A simple rule can be used to judge whether a result is significant or not. This is particularly useful in guarding against false positives. (ii) Scores can be compared with those from other types of search, such as sequence homol. (iii) Search parameters can be readily optimized by iteration. The strengths and limitations of probability-based scoring are discussed, particularly in the context of high throughput, fully automated protein identification.

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 7 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:342725 HCAPLUS
DOCUMENT NUMBER: 131:29562
TITLE: The potential use of laser capture microdissection to selectively obtain distinct populations of cells for proteomic **analysis.** Preliminary findings
AUTHOR(S): Banks, Rosamonde E.; Dunn, Michael J.; Forbes, Mary A.; Stanley, Anthea; **Pappin, Darryl**; Naven, Tom; Gough, Michael; Harnden, Patricia; Selby, Peter J.
CORPORATE SOURCE: ICRF Cancer Medicine Research Unit, St. James's Hospital, Leeds, LS9 7TF, UK
SOURCE: Electrophoresis (**1999**), 20(4-5), 689-700
CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Proteomics-based studies offer a powerful complementary approach to DNA/RNA-based investigations and are now being applied to investigate aspects of many diseases including cancer. The heterogeneous nature of tissue samples often makes interpretation difficult. The authors studied

the potential use of a novel laser capture microdissection (LCM) system to isolate cells of interest for subsequent proteomic **anal.** Retrieval of selected cells is achieved by activation of a transfer film placed in contact with a tissue section, by a laser beam (30 or 60 μm diameter) which is focused on a selected area of tissue using an inverted microscope. The precise area of film targeted by the laser bonds to the tissue beneath it and these cells are then lifted free of surrounding tissue. Although the technique was shown to be readily compatible with subsequent **anal.** of nucleic acids, little information is yet available regarding the application of protein-based **analyses** to the captured tissue. We report preliminary data regarding the potential use of the LCM system in combination with 2-D electrophoresis to examine protein profiles of selected tissue areas. Electrophoretic profiles of proteins from normal and malignant renal tissue samples showed little change following LCM, 9 selected proteins showed identical mass spectrometric sequencing profiles, and 2 selected proteins retained antigenicity. Dissection of epithelial tissue from a sample of normal human cervix resulted in enrichment of some proteins compared with **anal.** of the whole tissue. LCM will be a valuable adjunct to proteomic studies although further detailed validation is necessary.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 8 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:184612 HCAPLUS
DOCUMENT NUMBER: 131:41104
TITLE: Re-evaluation of the primary structure of Ralstonia eutropha phasin and implications for polyhydroxyalkanoic acid granule binding
AUTHOR(S): Hanley, Steven Zachary; **Pappin, Darryl J. C.**; Rahman, Dinah; White, Andrew J.; Elborough, Kieran M.; Slabas, Antoni R.
CORPORATE SOURCE: Department of Biological Sciences, University of Durham, Durham, DH13LE, UK
SOURCE: FEBS Letters (**1999**), 447(1), 99-105
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sequence **anal.** of several cDNAs encoding the phasin protein of Ralstonia eutropha indicated that the carboxyl terminus of the resulting derived protein sequence is different from that reported previously. This was confirmed by: (1) sequencing of the genomic DNA; (2) SDS-PAGE and peptide **anal.** of wild-type and recombinant phasin; and (3) mass spectrometry of wild-type phasin protein. The results have implications for the model proposed for the binding of this protein to polyhydroxyalkanoic acid granules in the bacterium.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 9 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:810503 HCAPLUS
DOCUMENT NUMBER: 128:100876
TITLE: HLA-DO is a negative modulator of HLA-DM-mediated MHC class II peptide loading
AUTHOR(S): van Ham, S. M.; Tjin, E. P. M.; Lillemeier, B. F.; Gruneberg, U.; van Meijgaarden, K. E.; Pastoors, L.; Verwoerd, D.; Tulp, A.; Canas, B.; Rahman, D.; Ottenhoff, T. H. M.; **Pappin, D. J. C.**; Trowsdale, J.; Neefjes, J.

CORPORATE SOURCE: Dep. Cellular Biochemistry, Netherlands Cancer Inst., Amsterdam, 1066 CX, Neth.
SOURCE: Current Biology (**1997**), 7(12), 950-957
CODEN: CUBLE2; ISSN: 0960-9822
PUBLISHER: Current Biology Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Class II mols. of the major histocompatibility complex become loaded with antigenic peptides after dissociation of invariant chain-derived peptides (CLIP) from the peptide-binding groove. The human leukocyte antigen (HLA)-DM is a prerequisite for this process, which takes place in specialized intracellular compartments. HLA-DM catalyzes the peptide-exchange process, simultaneously functioning as a peptide 'editor', favoring the presentation of stable binding peptides. Recently, HLA-DO, an unconventional class II mol., has been found associated with HLA-DM in B cells, yet its function has remained elusive. The function of the HLA-DO complex was investigated by expression of both chains of the HLA-DO heterodimer (either alone or fused to green fluorescent protein) in human Mel JuSo cells. Expression of HLA-DO resulted in greatly enhanced surface expression of CLIP via HLA-DR3, the conversion of class II complexes to the SDS-unstable phenotype and reduced antigen presentation to T-cell clones. **Anal.** of peptides eluted from HLA-DR3 demonstrated that CLIP was the major peptide bound to class II in the HLA-DO transfectants. Peptide exchange assays in vitro revealed that HLA-DO functions directly at the level of class II peptide loading by inhibiting the catalytic action of HLA-DM. Thus, HLA-DO is a neg. modulator of HLA-DM. By stably associating with HLA-DM, the catalytic action of HLA-DM on class II peptide loading is inhibited. HLA-DO thus affects the peptide repertoire that is eventually presented to the immune system by MHC class II mols.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:623392 HCAPLUS
DOCUMENT NUMBER: 127:306390
TITLE: Qa-1 interaction and T cell recognition of the Qa-1 determinant modifier peptide
AUTHOR(S): Cotterill, Lisa A.; Stauss, Hans J.; Millrain, Margaret M.; **Pappin, Darryl J. C.**; Rahman, Dinah; Canas, Benito; Chandler, Phillip; Stackpoole, Arthur; Simpson, Elizabeth; Robinson, Peter J.; Dyson, Julian P.
CORPORATE SOURCE: Royal Postgraduate Medical School, Hammersmith Hospital, London, W12 0NN, UK
SOURCE: European Journal of Immunology (**1997**), 27(9), 2123-2132
CODEN: EJIMAF; ISSN: 0014-2980
PUBLISHER: Wiley-VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The peptide-binding properties of the nonclassical major histocompatibility complex (MHC) class 1b mol. Qa-1 were investigated using a transfected hybrid mol. composed of the α1 and α2 domains of Qa-1b and the α3 domain of H-2Db. This allowed the use of a monoclonal antibody directed against H-2Db while retaining the peptide-binding groove of Qa-1b. By comparison with classical MHC class I mols., intracellular maturation of the chimeric mol. was inefficient with weak intracellular association with β2-microglobulin. However, at the cell surface the hybrid mols. were stably associated with

β2-microglobulin and were recognized by cytotoxic T lymphocyte (CTL) clones specific for the Qa-1b-presented peptide Qdm (AMAPRTLLL). A whole-cell binding assay was used to determine which residues of Qdm were important for binding to Qa-1b and CTL clones served to identify residues important for T cell recognition. Substitutions at position 1 and 5 did not reduce the efficiency of binding and had little effect on CTL recognition. In contrast, substitutions at position 9 resulted in loss of MHC class I binding. Mass spectrometric **anal.** of peptides eluted from immunopurified Qa-1b/ Db mols. indicated that Qdm was the dominant peptide. The closely related peptide, AMVPRTLLL, which is derived from the signal sequence of H-2Dk, was also present, although it was considerably less abundant. The mass profile suggested the presence of addnl. peptides the majority of which consisted of 8-10 amino acid residues. Finally, the finding that a peptide derived from Klebsiella pneumoniae can bind raises the possibility that this non-classical MHC class I mol. may play a role in the presentation of peptides of microorganisms.

L16 ANSWER 11 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:440822 HCAPLUS
DOCUMENT NUMBER: 127:201501
TITLE: p47 is a cofactor for p97-mediated membrane fusion
AUTHOR(S): Kondo, Hisao; Rabouille, Catherine; Newman, Richard; Levine, Timothy Pl; **Pappin, Darryl**; Freemont, Paul; Warren, Graham
CORPORATE SOURCE: Cell Biol. Lab., Imperial Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Nature (London) (**1997**), 388(6637), 75-78
CODEN: NATUAS; ISSN: 0028-0836
PUBLISHER: Macmillan Magazines
DOCUMENT TYPE: Journal
LANGUAGE: English
AB At least two distinct ATPases, NSF and p97, are known to be involved in the heterotypic fusion of transport vesicles with their target membranes and the homotypic fusion of membrane compartments. The NSF-mediated fusion pathway is the best characterized, many of the components having been identified and their functions **analyzed.** In contrast, none of the accessory proteins for the p97-mediated fusion pathway has been identified. Now the authors have identified the first such component a protein of relative mol. mass 47,000 (p47), which forms a tight stoichiometric complex with cytosolic p97 (one trimer of p47 per hexamer of p97). It is essential for the p97-mediated regrowth of Golgi cisternae from mitotic Golgi fragments, a process restricted to animal cells. As a homolog of p47 exists in budding yeast, this indicates that it might also be involved in other membrane fusion reactions catalyzed by p97, such as karyogamy.

L16 ANSWER 12 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:109668 HCAPLUS
DOCUMENT NUMBER: 126:222454
TITLE: **Analysis** of DNA by "charge tagging" and matrix-assisted laser desorption/ionization mass spectrometry
AUTHOR(S): Gut, Ivo G.; Jeffery, William A.; **Pappin, Darryl J. C.**; Beck, Stephan
CORPORATE SOURCE: DNA Sequencing Laboratory, Imperial Cancer Research Fund, London, WC2A 3PX, UK
SOURCE: Rapid Communications in Mass Spectrometry (**1997**), 11(1), 43-50
CODEN: RCMSEF; ISSN: 0951-4198

PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have developed a method to quant. attach quaternary ammonium fixed charge tags to the 5' or 3'NH2 ends of DNA using N-hydroxysuccinimidyl ester chemical The chemical conditions for tagging were chosen so that tagging takes place exclusively on aliphatic NH2 groups while base amino groups remain unmodified. The charge tagging chemical was combined with a previously developed backbone alkylation procedure for phosphorothioate DNA. The efficiency of the detection in matrix-assisted laser desorption/ionization (MALDI) mass spectrometry of unmodified and modified DNA (phosphorothioate backbone, charge tagged, backbone alkylated, and charge tagged and backbone alkylated) was investigated using a series of different matrixes. For α-cyano-4-hydroxycinnamic acid (a matrix, commonly used for the **anal.** of proteins, but which gives unsatisfactory results with unmodified DNA). For instance, the charge tagged and backbone alkylated DNA is detectable with a sensitivity and resolution comparable with that for peptides. The combination of charge tagging and backbone alkylation with the use of a suitable matrix improves the detectability of small oligonucleotides by MALDI by a factor greater than 100 compared to unmodified oligonucleotides.
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 13 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:37513 HCAPLUS
DOCUMENT NUMBER: 126:56960
TITLE: Peptide mass fingerprinting using MALDI-TOF mass spectrometry
AUTHOR(S): **Pappin, Darryl J. C.**
CORPORATE SOURCE: Protein Isolation and Cloning Lab, Imperial Cancer Research Fund, London, UK
SOURCE: Methods in Molecular Biology (Totowa, New Jersey) (**1997**), 64(Protein Sequencing Protocols), 165-173
CODEN: MMBIED; ISSN: 1064-3745
PUBLISHER: Humana
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The protocols of the title method which permit reliable peptide maps to be obtained from subpicomole quantities of material are described.

L16 ANSWER 14 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:398529 HCAPLUS
DOCUMENT NUMBER: 125:109439
TITLE: Identification of myocardial proteins from two-dimensional gels by database matching of proteolytic peptide masses
AUTHOR(S): Sutton, Chris W.; Pemberton, Kay S.; Cottrell, John S.; Corbett, Joseph M.; Wheeler, Colin H.; Dunn, Michael J.; **Pappin, Darryl J.**
CORPORATE SOURCE: Finnigan MAT Ltd., HP2 4TG, UK
SOURCE: Perspectives on Protein Engineering & Complementary Technologies, Collected Papers, International Symposium, 3rd, Oxford, Sept. 13-17, 1994 (**1995**), Meeting Date 1994, 82-85. Editor(s): Geisow, Michael J.; Epton, Roger. Mayflower Worldwide: Kingswinford, UK.
CODEN: 62ZQAP
DOCUMENT TYPE: Conference

LANGUAGE: English
AB Two-dimensional gels offer the most powerful method for separating complex protein mixts., but subsequent methods for **analyzing** individual components are slow. The identification of proteins can be accelerated by using a combination of protease digest and MALDI MS. The peptide mass spectrum of a protein represents a unique fingerprint defined by the amino acid sequence and the properties of the protease. Software has been developed so that individual peptide masses can be used to search a mass-based peptide database generated from established protein sequence databases. A list of the closest matching proteins is produced to allow identification of the sample. Examples of myocardial tissue proteins separated by 2D gel electrophoresis and identified by mass peptide fingerprinting are used to illustrate this strategy.

L16 ANSWER 15 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:159514 HCAPLUS
DOCUMENT NUMBER: 124:225544
TITLE: Peptide-mass fingerprinting as a tool for the rapid identification and mapping of cellular proteins
AUTHOR(S): **Pappin, D. J. C.**; Rahman, D.; Hansen, H. F.; Jeffery, W.; Sutton, C. W.
CORPORATE SOURCE: Imperial Cancer Research Fund, London, WC2A 3PX, UK
SOURCE: Methods in Protein Structure Analysis, [Proceedings of the International Conference on Methods in Protein Structure Analysis], 10th, Snowbird, Utah, Sept. 8-13, 1994 (**1995**), Meeting Date 1994, 161-73.
Editor(s): Atassi, M. Zouhair; Appella, Ettore.
Plenum: New York, N. Y.
CODEN: 62LPAK
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Simplified digestion methods based on the use of octyl glucoside that allow for the rapid, single step digestion of electro-blotted proteins in a form suitable for both **anal.** by MALD spectroscopy or conventional Edman micro-sequencing are described.

L16 ANSWER 16 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:14825 HCAPLUS
DOCUMENT NUMBER: 124:76689
TITLE: Identification of phosphorylation sites in the mouse estrogen receptor
AUTHOR(S): Lahooti, H.; White, R.; Hoare, S. A.; Rahman, D.; **Pappin, D. J. C.**; Parker, M. G.
CORPORATE SOURCE: Mol. Endocrinology and Protein Sequencing Lab., Imperial Cancer Research Fund, London, WC2A 3PX, UK
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (**1995**), 55(3/4), 305-13
CODEN: JSBBEZ; ISSN: 0960-0760
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Phosphorylation sites in the mouse estrogen receptor, expressed in COS-1 cells in the presence of 17β-estradiol, have been mapped by solid phase microsequencing. The receptor was first radiolabeled with [32P]orthophosphate and a number of 3H- or 14C-labeled amino acids, immunopurified and then tryptic peptides were separated by thin layer chromatog. or high performance liquid chromatog. Amino acid sequence **anal.** indicated that Ser-122, Ser-156, Ser-158 and Ser-298 were phosphorylated. The substitution of Ser-122 and Ser-298 with alanine had a negligible effect on the transcriptional activity of the receptor in

transfected cells. However, a reduction of transcriptional activity was observed
when Ser-122 was mutated in the context of mutations in a putative amphipathic α-helix involved in AF-2 activity. Thus, a region of AF-1 that encompasses Ser-122 appears to interact with AF-2 in the full length receptor.

L16 ANSWER 17 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:936888 HCAPLUS
DOCUMENT NUMBER: 124:224652
TITLE: The myristoylated alanine-rich C-kinase substrate (MARCKS) is sequentially phosphorylated by conventional, novel and atypical isotypes of protein kinase C
AUTHOR(S): Herget, Thomas; Oehrlein, Silke A.; **Pappin, Darryl J. C.**; Rozengurt, Enrique; Parker, Peter J.
CORPORATE SOURCE: Institute of Physiological Chemistry, University of Mainz, Mainz, D-55099, Germany
SOURCE: European Journal of Biochemistry (**1995**), 233(2), 448-57
CODEN: EJBCAI; ISSN: 0014-2956
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The myristoylated Ala-rich C-kinase substrate (MARCKS) is the major protein kinase C (PKC) substrate in many cell types including fibroblasts and brain cells. The phosphorylation of MARCKS and the site specificity for different PKC isotypes are described. Conventional (c)PKC β1, novel (n)PKC δ and nPKC ε efficiency phosphorylated the MARCKS protein in vitro. The Km values were extremely low, reflecting a high affinity between kinases and substrate. The apparent affinity of nPKC δ (Km = 0.06 μM) was higher than that of nPKC ε and cPKC β1 (Km = 0.32 μM). The rate of substrate phosphorylation was inversely correlated with affinity and decreased in the oder nPKC ε > cPKC β1 > nPKC δ. Atypical (a)PKC ζ did not phosphorylate the intact MARCKS protein. However, a 25-amino-acid peptide deduced from the MARCKS phosphorylation domain, was efficiently phosphorylated by aPKC ζ as well as by the other three PKC. Site **anal.** revealed that only Ser residues S152, S156 and S163 were phosphorylated, with S163 phosphorylated highest, followed by S156 and S152; in contrast, S160 and S167 were not phosphorylated. No further PKC phosphorylation sites could be detected in MARCKS. The phosphorylation pattern was independent of the type of PKC isotype used. Kinetic **anal.** showed, that MARCKS is sequentially phosphorylated in the order S156 > S163 > S152 by cPKC, nPKC and aPKC. There was no dramatic difference in the sequential phosphorylation of MARCKS detectable when comparing the 4 PKC isotypes. The results are discussed in the context of the functional significance of MARCKS phosphorylation.

L16 ANSWER 18 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:491256 HCAPLUS
DOCUMENT NUMBER: 122:234807
TITLE: Identification of myocardial proteins from two-dimensional gels by peptide mass fingerprinting
AUTHOR(S): Sutton, Chris W.; Pemberton, Kay S.; Cottrell, John S.; Corbett, Joseph M.; Wheeler, Colin H.; Dunn, Michael J.; **Pappin, Darryl J.**
CORPORATE SOURCE: Finnigan MAT Ltd., Hempstead, UK
SOURCE: Electrophoresis (**1995**), 16(3), 308-16

CODEN: ELCTDN; ISSN: 0173-0835
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two-dimensional gels offer a powerful method for separating complex protein mixts., but subsequent methods for **analyzing** individual components, such as protein sequencing and Western immunoblotting, are laborious and slow. The identification of proteins can be accelerated by using a combination of protease digestion and matrix assisted laser desorption-mass spectrometry (MALDI-MS). The peptide mass spectrum of a protein represents a unique fingerprint determined by the amino acid sequence and the cleavage properties of the protease. Software has been developed so that peptide masses can be used to search a mass-based peptide database generated from established protein sequence databases. A list of the closest matching proteins is produced to allow identification of the sample. The strategy was applied to 52 protein spots from human myocardial tissue separated by two-dimensional electrophoresis (2-DE) gels and **analyzed** blind. Conditions for optimal trypsin digestion of proteins electroblotted onto polyvinylidene difluoride (PVDF) membranes are described. Mass data were generated from both Coomassie Brilliant Blue and sulforhodamine B-stained proteins, though the former required destaining prior to digestion. Alkylation of cysteine and oxidation of methionine were significant modifications that influenced the successful identification of a protein spot. Examples are presented to illustrate the advantages and disadvantages of this approach.

L16 ANSWER 19 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:675783 HCAPLUS
DOCUMENT NUMBER: 121:275783
TITLE: Peptide ladder sequencing by mass spectrometry using a novel, volatile degradation reagent
AUTHOR(S): Jones, Michael Bartlet; Jeffrey, William A.; Hansen, Hans F.; **Pappin, Darryl J. C.**
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Rapid Communications in Mass Spectrometry (**1994**), 8(9), 737-42
CODEN: RCMSEF; ISSN: 0951-4198
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A conceptually novel approach to protein sequencing involves the generation of ragged-end polypeptide chains followed by mass spectroscopic **anal.** of the resulting nested set of fragments. We report here on the synthesis and development of a volatile isothiocyanate (trifluoroethylisothiocyanate) that allows the identification of several consecutive residues starting with a few picomoles of peptide. The nested set of peptides is generated simply by adding equal aliquots of starting peptide each cycle and driving both the coupling and cleavage reactions to completion. No addnl. reagents are required to act as chain terminators and retention of the peptide terminal amine allows for subsequent modification with quaternary ammonium alkyl NHS esters to improve sensitivity. Complex washing procedures are not required each cycle, as reagents and byproducts are efficiently removed under vacuum, eliminating extractive loss. Multiple peptide samples can be proposed simultaneously, with each degradation cycle completed in 35-40 min. The inherent simplicity of the process should allow for easy automation and permit rapid processing of samples in parallel.

L16 ANSWER 20 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:647959 HCAPLUS

DOCUMENT NUMBER: 121:247959
TITLE: Competition between nuclear localization and secretory signals determines the subcellular fate of a single CUG-initiated form of FGF3
AUTHOR(S): Kiefers, Paul; Acland, Piers; **Pappin, Darryl** ; Peters, Gordon; Dickson, Clive
CORPORATE SOURCE: Imperial Cancer Research Lund, London, WC2A 3PX, UK
SOURCE: EMBO Journal (**1994**), 13(17), 4126-36
CODEN: EMJODG; ISSN: 0261-4189
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The presumed open reading frame for mouse FGF3, starting at the most 5' AUG codon, predicts a hydrophobic N-terminus characteristic of a signal peptide for secretion. However, in reticulocyte lysates and transfected COS-1 cells, the full-length Fgf-3 cDNA is translated almost exclusively from an upstream CUG codon. The resultant products are distributed in both the nucleus and the secretory pathway, implying that the single CUG-initiated form of FGF3 has dual fates. By **analyzing** a series of deletion and replacement mutants and by linking parts of FGF3 to a heterologous protein, we show that secretion is mediated by cleavage adjacent to the previously defined signal peptide, whereas nuclear localization is determined primarily by a classical but relatively weak bipartite motif. In the context of FGF3, nuclear localization also requires the N-terminal sequences which lie upstream of the signal peptide. Thus, the subcellular fate of FGF3 is determined by the competing effects of signals for secretion and nuclear localization within the same protein, rather than by alternative initiation or processing.

L16 ANSWER 21 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1994:75401 HCAPLUS
DOCUMENT NUMBER: 120:75401
TITLE: Tyrosine phosphorylation of α tubulin in human T lymphocytes
AUTHOR(S): Ley, Steven C.; Verbi, Winston; **Pappin, Darryl J. C.**; Druker, Brian; Davies, Adelina A.; Crumpton, Michael J.
CORPORATE SOURCE: Natl. Inst. Med. Res., London, UK
SOURCE: European Journal of Immunology (**1994**), 24(1), 99-106
CODEN: EJIMAF; ISSN: 0014-2980
DOCUMENT TYPE: Journal
LANGUAGE: English

AB N-terminal sequencing of the 55- and 50-kDa polypeptides affinity purified on a phosphotyrosine monoclonal antibody column from activated Jurkat T cells identified α and β tubulin. Two-dimensional gel **anal.** indicated that α tubulin was directly phosphorylated on tyrosine. β Tubulin was not detectably tyrosine phosphorylated but was precipitated by anti-phosphotyrosine (PTyr) antibody by virtue of its association with the α subunit as a heterodimer. Phosphotyrosyl α tubulin was not incorporated into intact microtubules and was all in the unpolymd. soluble fraction. Thus, tyrosine phosphorylation of α tubulin may inhibit the ability of this subunit to polymerize into microtubules. Stimulation of Jurkat T cells via T cell receptor increased the amount of tubulin precipitated by the anti-PTyr antibody. These data raise the possibility that the polymerization of tubulin heterodimers may be regulated by phosphorylation on tyrosine during T cell activation.

L16 ANSWER 22 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:644768 HCAPLUS

DOCUMENT NUMBER: 119:244768
TITLE: Rapid indentification of proteins by peptide-mass fingerprinting. [Erratum to document cited in CA119(15):155221x]
AUTHOR(S): **Pappin, D. J.**; Hojrup, P.; Bleasby, A. J.
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Current Biology (**1993**), 3(7), 487
CODEN: CUBLE2; ISSN: 0960-9822
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The errors were not reflected in the abstract or the index entries.

L16 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:555221 HCAPLUS
DOCUMENT NUMBER: 119:155221
TITLE: Rapid indentification of proteins by peptide-mass fingerprinting
AUTHOR(S): **Pappin, D. J. C.**; Hojrup, P.; Bleasby, A. J.
CORPORATE SOURCE: Protein Sequencing Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Current Biology (**1993**), 3(6), 327-32
CODEN: CUBLE2; ISSN: 0960-9822
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The authors report the development of the mol. weight search (MOWSE) peptide-mass database at the SERC Daresbury Laboratory Practical experience showed that sample proteins can be identified uniquely from as few as 3 or 4 exptl. determined peptide masses when these are screened against a fragment database that is derived from >50,000 proteins. Peptide-mass fingerprints can prove as discriminating as linear peptide sequences but can be obtained in a fraction of the time using less protein. In many cases, this allows for a rapid identification of a sample protein before committing it to protein sequence **anal.** Fragment masses also provide information, at the protein level, that is complementary to the information provided by large-scale DNA sequencing or mapping projects.

L16 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:581148 HCAPLUS
DOCUMENT NUMBER: 115:181148
TITLE: Purification and characterization of biologically active scatter factor from ras-transformed NIH 3T3 conditioned medium
AUTHOR(S): Coffer, Arnold; Fellows, Jane; Young, Susan; **Pappin, Darryl**; Rahman, Dinah
CORPORATE SOURCE: Protein Isol. Cloning Lab., Imp. Cancer Res. Fund, London, WC2A 3PX, UK
SOURCE: Biochemical Journal (**1991**), 278(1), 35-41
CODEN: BIJOAK; ISSN: 0306-3275
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Scatter factor (SF), a glycoprotein produced by cultured fibroblasts, acts in vitro on epithelial cells causing separation and increased local motility. In this study, the polypeptide was purified to apparent homogeneity in high yields with conserved biol. activity from medium conditioned by ras-transformed NIH 3T3 cells, by a 3-step procedure involving ammonium sulfate fractionation, cation-exchange, and hydroxyapatite chromatog. After purification, SF specific activity increased from .apprx.0.3 units/μg in unprocessed conditioned medium to .apprx.5 units/ng, and cumulative recovery of biol. activity was .apprx.38%. Treatment of pure SF with

N-glycanase resulted in a decreased Mr, but no concomitant effect was observed on biol. activity. Proteolytic activity was absent from samples of both partially purified and pure SF. The biochem. studies showed that SF, which is highly aggregated in low-ionic-strength media, is not aggregated in 0.4 M-salt. Under non-reducing conditions, pure SF migrated as a single strained band at Mr 67,000 on SDS/PAGE, and biol. activity was eluted from unstained gels with an identical Mr. SF was electrofocused sharply at pI 8.5 with no degradation of activity. From ultracentrifugation studies (under non-aggregating conditions), the sedimentation coefficient of active SF was 3.7S and f.p.l.c. mol. sieve chromatog. indicated a Stokes' radius of 2.95 nm. The calculated Mr from these data was 61,400. The appearance of 3 stained polypeptides of Mr 82,000, 57,000, and 32,000 derived from the Mr-67,000 constituent after reduction with mercaptoethanol suggests that SF may be a heterodimer of Mr-57,000 and -32,000 subunits. Data from protein sequence **anal.** of the hydroxyapatite-purified protein confirms that SF has sequence identity with both rat hepatocyte growth factor and human fibroblast tumor cytotoxic factor.

L16 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:467672 HCAPLUS
DOCUMENT NUMBER: 115:67672
TITLE: New approaches to covalent sequence **analysis**
AUTHOR(S): **Pappin, Darryl J. C.**; Coull, James M.; Koester, Hubert
CORPORATE SOURCE: MilliGen/Biosearch Div., Millipore, Burlington, MA, 01803, USA
SOURCE: Curr. Res. Protein Chem.: Tech., Struct., Funct., [Pap. Annu. Symp. Protein Soc.], 3rd (**1990**), Meeting Date 1989, 191-202. Editor(s): Villafranca, Joseph J. Academic: San Diego, Calif.
CODEN: 56XQAW
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report on covalent (solid-phase) sequence **anal.** of proteins. Thus, peptides or proteins are blotted onto an underivatized polyvinylidene membranes, stained by conventional techniques, and then efficiently covalently immobilized to the membrane surface by entrapment in a thin polymer coating.

L16 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:425568 HCAPLUS
DOCUMENT NUMBER: 115:25568
TITLE: Immobilization of proteins and peptides on insoluble supports for sequencing and other applications
INVENTOR(S): **Pappin, Darryl J. C.**; Coull, James M.; Koester, Hubert
PATENT ASSIGNEE(S): Millipore Corp., USA
SOURCE: Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 410323	A2	19910130	EP 1990-113972	19900720 <--
EP 410323	A3	19920408		
R: DE, FR, GB, IT, NL, SE				
US 5071909	A	19911210	US 1989-385711	19890726 <--

JP 03141300 A2 19910617 JP 1990-194113 19900724 <--
PRIORITY APPLN. INFO.: US 1989-385711 A 19890726
AB A peptide or protein is immobilized onto a flat, microporous membrane by (1) adsorbing the peptide or protein and a crosslinkable polymer onto the membrane surface, and (2) crosslinking the polymer to produce a polymer network entrapping the protein or peptide therein. The immobilized peptide or protein is suitable for sequence **anal.** or other chemical or enzymic processes. Thus, a polyvinylidene difluoride membrane disk containing electroblotted β-lactoglobulin A and stained with sulforhodamine B was treated with diisopropyl-carbodiimide and methylenedianiline (polymer crosslinking agent), dried, then treated with polyacrylic acid (5000 mol. weight). The prepared disk was subjected to 20 cycles of Edman degradation The initial sequencing yield was 35 pmol and the repetitive yield 90%.

L16 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:243669 HCAPLUS
DOCUMENT NUMBER: 114:243669
TITLE: Functionalized membrane supports for covalent protein microsequence **analysis**
AUTHOR(S): Coull, James M.; **Pappin, Darryl J. C.**; Mark, Jonathan; Aebersold, Ruedi; Koster, Hubert
CORPORATE SOURCE: MilliGen/Bios., Div. Millipore, Burlington, MA, 01803, USA
SOURCE: Analytical Biochemistry (**1991**), 194(1), 110-20
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Methods were developed for high-yield covalent attachment of peptides and proteins to isothiocyanate and arylamine-derivatized poly(vinylidene difluoride) membranes for solid-phase sequence **anal.** Solns. of protein or peptide were dried onto 8-mm membrane disks such that the functional groups on the surface and the polypeptide were brought into close proximity. In the case of the isothiocyanate membrane, reaction between polypeptide amino groups and the surface isothiocyanate moieties was promoted by application of aqueous N-methylmorpholine. Attachment of proteins and peptides to the arylamine surface was achieved by application of water-soluble carbodiimide in a pH 5.0 buffer. Edman degradation of covalently bound polypeptides was accomplished with initial and repetitive sequence yields ranging 33-75% and 88.5-98.5%, resp. The yields were independent of the sample load (20 pmol to >1 nmol) for either surface. Significant loss of material was not observed when attachment residues were encountered during sequence runs. Application of bovine β-lactoglobulin A chain, staphylococcus protein A, or the peptide melittin to the isothiocyanate membrane allowed for extended N-terminal sequence identification (35 residues from 20 pmol of β-lactoglobulin). Several synthetic and naturally occurring peptides were sequenced to the C-terminal residue following attachment to the arylamine surface. In 1 example, 10 μg of bovine α-casein was digested with staphylococcal protease V8 and the peptides were separated by reversed-phase chromatog. Peptide fractions were then directly applied to arylamine membrane disks for covalent sequence **anal.** From as little as 2 pmol of initial signal it was possible to determine substantial sequence information (>10 residues).

L16 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:420480 HCAPLUS
DOCUMENT NUMBER: 113:20480
TITLE: Solid-phase sequence **analysis** of proteins

electroblotted or spotted onto polyvinylidene difluoride membranes
AUTHOR(S): **Pappin, Darryl J. C.**; Coull, James M.; Koster, Hubert
CORPORATE SOURCE: MilliGen/Biosearch, Burlington, MA, 01803, USA
SOURCE: Analytical Biochemistry (**1990**), 187(1), 10-19
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Electroblotted proteins noncovalently bound to polyvinylidene difluoride (PVDF) membranes are typically sequenced using adsorptive sequencer protocols (gas phase or pulsed-liquid) that do not require a covalent linkage between protein and surface. Simple chemical protocols were developed where proteins are first electroblotted onto unmodified PVDF membranes, visualized with common protein stains, and then immobilized for solid-phase sequence **anal.** Adsorbed, stained proteins are first treated with phenylisothiocyanate (PITC) to modify α and ε amines. The protein is then overlayed with a solution of 1,4-phenylene diisothiocyanate (DITC), followed by a few microliters of a basic solution containing a poly(alkylamine). As the polymer dries onto the surface both polymer and remaining protein amino groups are crosslinked by DITC. The protein is thus immobilized to the membrane surface by entrapment in a thin polymer coating. The coating is transparent to the degradation chemical, and extensive enough to remain immobilized even in the absence of any covalent link between polymer and surface. Partial modification with PITC allows for identification of N-terminal and internal lysine residues during sequencing. The process was tested with a variety of poly(alkylamines), linear and branched, with mol. wts. ranging from 600 to >100,000. Proteins bound in this manner were successfully sequenced using covalent (solid-phase) sequencer protocols with cyclic times as short as 26 min.

L16 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:113201 HCAPLUS
DOCUMENT NUMBER: 112:113201
TITLE: The extrinsic 33 kDa polypeptide of the oxygen-evolving complex of photosystem II is a putative calcium-binding protein and is encoded by a multi-gene family in pea
AUTHOR(S): Wales, Richard; Newman, Barbara J.; **Pappin, Darryl**; Gray, John C.
CORPORATE SOURCE: Bot. Sch., Univ. Cambridge, Cambridge, CB2 3EA, UK
SOURCE: Plant Molecular Biology (**1989**), 12(4), 439-51
CODEN: PMBIDB; ISSN: 0167-4412
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The extrinsic 33 kDa polypeptide of the water-oxidizing complex has been extracted from pea photosystem II particles by washing with alkaline-Tris and purified by ion-exchange chromatog. The N-terminal amino acid sequence has been determined, and specific antisera have been raised in rabbits and used to screen a pea leaf cDNA library in λgt 11. Determination of the nucleotide sequence of pos. clones revealed an essentially full-length cDNA for the 33 kDa polypeptide, the deduced amino acid sequence showing it to code for a mature protein of 248 amino acids with an N-terminal transit peptide of 81 amino acids. The protein showed a high degree of conservation with previously reported sequences for the 33 kDa protein from other species and the sequence contained a putative Ca2+-binding site with homol. to mammalian intestinal calcium-binding proteins. Northern

anal. of total pea RNA indicated a message of approx. 1.4 kb, in good agreement with the size of the cDNA obtained at indicated a message of approx. 1.4 kb, in good agreement with the size of the cDNA obtained at 1.3 kbp. Southern blots of genomic DNA probed with the labeled cDNA give rise to several bands suggesting that the 33 kDa polypeptide is coded by a multi-gene family.

L16 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1989:611670 HCAPLUS
DOCUMENT NUMBER: 111:211670
TITLE: Exported proteins of Neurospora crassa: 1-glucoamylase
AUTHOR(S): Koh-Luar, Siok Im; Parish, J. H.; Bleasby, A. J.; **Pappin, D. J. C.**; Ainley, K.; Johansen, F. E.; McPherson, M. J.; Radford, A.
CORPORATE SOURCE: Dep. Biochem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Enzyme and Microbial Technology (**1989**), 11(10), 692-5
CODEN: EMTED2; ISSN: 0141-0229
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Polypeptides were extracted from the culture supernatants of N. crassa growing in a variety of media. The polypeptides were **analyzed** by quant. SDS-PAGE and the single polypeptide produced in the largest amount under the conditions tested was of mol. weight 69,000 and was referred to as p69. The synthesis of p69 was induced by starch and maltose, and studies on a partially purified preparation established that it was a glucoamylase. The sequence of the N-terminal 30 amino acids of p69 showed that this was related to sequences of amylases from Aspergillus species. A synthetic oligonucleotide probe was synthesized and used to search for the corresponding gene(s) in Neurospora. A unique region was identified and mapped in a clone from a genomic library. The implications of the work for the development of Neurospora export and expression systems are discussed.

L16 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:625726 HCAPLUS
DOCUMENT NUMBER: 109:225726
TITLE: Amino acid sequence **analysis** of the small subunit of ribulose bisphosphate carboxylase from Fucus (Phaeophyceae)
AUTHOR(S): Keen, Jeffrey N.; **Pappin, Darryl J. C.**; Evans, Leonard V.
CORPORATE SOURCE: Dep. Pure Appl. Biol., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Journal of Phycology (**1988**), 24(3), 324-7
CODEN: JPYLAJ; ISSN: 0022-3646
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Amino acid sequence information for the small subunit of ribulose 1,5-bisphosphate carboxylase/oxygenase (Rubisco) from a nongreen alga was reported. N-terminal sequences are presented for the polypeptide from three species of the genus Fucus (Phaeophyceae). Although homologous to small subunit polypeptides from other organisms, the Fucus sequences exhibit a unique N-terminal section resembling neither cyanobacterial nor chlorophytic sequences. This difference may be a consequence of the plastid DNA coding arrangement for the small subunit in chromophytes, a situation reported for the related organism Olisthodiscus but not previously investigated at the amino acid sequence level.

L16 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:182407 HCAPLUS
DOCUMENT NUMBER: 108:182407
TITLE: Isolation and characterization of a minor legumin and its constituent polypeptides from Pisum sativum (pea)
AUTHOR(S): March, John F.; **Pappin, Darryl J. C.**; Casey, Rod
CORPORATE SOURCE: John Innes Inst., Norwich, NR4 7UH, UK
SOURCE: Biochemical Journal (**1988**), 250(3), 911-15
CODEN: BIJOAK; ISSN: 0306-3275
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The purification and characterization of a minor legumin species from P. sativum is described. Electrophoretic data indicate that it corresponds to a legumin subunit pair previously designated L1. The β-polypeptides of the minor legumin have a phenylalanine N-terminus. This is the first time that an amino acid other than glycine has been reported as the N-terminus of the basic polypeptides from legumin-like proteins from any plant species. Sequence **analyses** of the isolated α- and β-polypeptides of the minor legumin show that it does not correspond to any of the 3 legumin gene families previously defined on the basis of DNA hybridiations and genetic **analyses.**

L16 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:147347 HCAPLUS
DOCUMENT NUMBER: 108:147347
TITLE: N-terminal amino acid sequence **analysis** of the subunits of pea photosystem I
AUTHOR(S): Dunn, Paul P. J.; Packman, Leonard C.; **Pappin, Darryl**; Gray, John C.
CORPORATE SOURCE: Dep. Bot., Univ. Cambridge, Cambridge, CB2 1QW, UK
SOURCE: FEBS Letters (**1988**), 228(1), 157-61
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Six core subunits of pea photosystem I were isolated and their N-terminal amino acid sequences determined by gas-phase or solid-phase sequencing. On average >30 residues were determined from the N-terminus of each polypeptide. Sequence **anal.** revealed three polypeptides with charged N-terminal regions (21, 17 and 11 kDa subunits), one polypeptide with a predominantly hydrophobic N-terminal region (9 kDa subunit), one polypeptide which is cysteine-rich (8 kDa subunit) and one which is alanine-rich (13 kDa subunit).

L16 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:191404 HCAPLUS
DOCUMENT NUMBER: 106:191404
TITLE: Homology between the pyrazine-binding protein from nasal mucosa and major urinary proteins
AUTHOR(S): Cavaggioni, A.; Sorbi, R. T.; Keen, J. N.; **Pappin, D. J. C.**; Findlay, J. B. C.
CORPORATE SOURCE: Ist. Fisiol., Univ. Parma, Parma, 43100, India
SOURCE: FEBS Letters (**1987**), 212(2), 225-8
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sequence **anal.** of the pyrazine-binding protein from bovine olfactory mucosa reveals marked homol. with a family of proteins of unknown function found in the urine of the adult male mouse and rat. In view of the dramatic biol. responses to odorants transmitted in male

rodent urines, it is proposed that these proteins play important roles in some aspects of odor transmission and reception.

L16 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:203984 HCAPLUS
DOCUMENT NUMBER: 104:203984
TITLE: Posttranslational processing of concanavalin A precursors in jackbean cotyledons
AUTHOR(S): Bowles, Dianna J.; Marcus, Susan E.; **Pappin, Darryl J. C.**; Findlay, John B. C.; Eliopoulos, Elias; Maycox, Peter R.; Burgess, Jeremy
CORPORATE SOURCE: Dep. Biochem., Univ. Leeds, Leeds, LS2 9JT, UK
SOURCE: Journal of Cell Biology (**1986**), 102(4), 1284-97
CODEN: JCLBA3; ISSN: 0021-9525
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Metabolic labeling of immature jackbean cotyledons with 14C-amino acids was used to determine the processing steps involved in the assembly of concanavalin A. Pulse-chase expts. and **analyses** of immunopptd. lectin forms indicated a complex series of events involving 7 distinct species. The structural relatedness of all of the intermediate species was confirmed by 2-dimensional mapping of 125I-tryptic peptides. An initial glycosylated precursor was deglycosylated and cleaved into smaller polypeptides, which subsequently reannealed over a period of 10-27 h. NH2-terminal sequencing of the abundant precursors confirmed that the intact subunit of concanavalin A was formed by the reannealing of 2 fragments, since the alignment of residues 1-118 and 119-237 was reversed in the final form of the lectin identified in the chase and the precursor first labeled. When the tissue was pulse-chased in the presence of monensin, processing of the glycosylated precursor was inhibited. The weak bases NH4Cl and chloroquine were without effect. Immunocytochem. studies showed that monensin treatment caused the accumulation of immunoreactive material at the cell surface and indicated that the ionophore had induced the secretion of a component normally destined for deposition within the protein bodies. Consideration of the tertiary structure of the glycosylated precursor and mature lectin showed that the entire series of processing events could occur without significant refolding of the initial translational product. Proteolytic events included removal of a peptide from the surface of the precursor mol. that connected the NH2- and COOH-termini of the mature protein. This processing activated the carbohydrate-binding activity of the lectin. The chase data suggested the occurrence of a simultaneous cleavage and formation of a peptide bond, raising the possibility that annealment of the fragments to give rise to the mature subunit involves a transpeptidation event rather than cleavage and subsequent religation.

L16 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:164913 HCAPLUS
DOCUMENT NUMBER: 104:164913
TITLE: Coronavirus IBV glycopolypeptides: locational studies using proteases and saponin, a membrane permeabilizer
AUTHOR(S): Cavanagh, David; Davis, Philip J.; **Pappin, Darryl J. C.**
CORPORATE SOURCE: Houghton Poultry Res. Statn., Houghton/Huntingdon/Cambs., PE17 2DA, UK
SOURCE: Virus Research (**1986**), 4(2), 145-56
CODEN: VIREDF; ISSN: 0168-1702
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [35S]methionine-labeled avian infectious bronchitis virus (IBV) (strain 41) and its purified protein components and virions of IBV-Beaudette were incubated with 10 proteases. Several proteases hydrolyzed all or some of the membrane glycopolypeptide M (mol. weight 30 kilodaltons [30K]) and removed .apprx.1.3K of peptide from the N terminus plus both glycans, as determined by SDS-polyacrylamide gel electrophoresis. N-terminal **anal** . of [3H]isoleucine-labeled M after hydrolysis by bromelain revealed that the first 9 residues were removed. After the virions were permeabilized with saponin, a further 2.5K decrease in mol. weight was produced from the C terminus. When considered with the hydropathicity plot **anal.** of the amino acid sequence of M, as few as 9-20 N-terminal amino acids may protrude at the outer membrane surface, and that there msy be a highly protease sensitive sequence of .apprx.20-25 residues at the C-terminus of M exposed in the lumen of the virion. S2 but not S1 was cleaved to a major glycopolypeptide of .apprx.71K by several proteases, and to 76K by trypsin. N-terminal sequencing of the 71K glycopolypeptide revealed that it had the same N terminus as intact S2. After hydrolysis in the presence and absence of saponin, it was concluded that S2 is very sensitive to hydrolysis near its C terminus at residues close to the outer membrane surface.

L16 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:590791 HCAPLUS
DOCUMENT NUMBER: 103:190791
TITLE: The primary sequence of Ricinus communis agglutinin. Comparison with ricin
AUTHOR(S): Roberts, Lynne M.; Lamb, F. Ian; **Pappin, Darryl J. C.**; Lord, J. Michael
CORPORATE SOURCE: Dep. Biol. Sci., University of Warwick, Coventry, CV4 7AL, UK
SOURCE: Journal of Biological Chemistry (**1985**), 260(29), 15682-6
CODEN: JBCHA3; ISSN: 0021-9258
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A mixture of synthetic oligonucleotides representing all possible sequences of a peptide present in the ricin B chain was used to screen a cDNA library constructed using ripening castor bean seed poly(A+) RNA. The 8 largest recombinant plasmids selected, by hybridization, a single mRNA species that encoded preprolectin, as shown by immunopptn. Restriction enzyme **anal.** of these clones showed 2 classes of sequences complementary to 2 distinct, but closely related, preprolectin mRNA species. The nucleotide sequence of the cloned cDNA from 1 of these classes encodes preproricin and has been presented elsewhere. The nucleotide sequence of the 2nd class is presented and represents the preproagglutinin of R. communis. The entire coding sequence was deduced from 2 overlapping cDNA clones with inserts of 1668 and 1151 base pairs. The coding region defines a preproprotein with a 24-amino acid N-terminal signal sequence preceding the A chain (266 amino acids) which is joined to the B chain (262 amino acids) by a 12-amino acid linking peptide. The protein was confirmed as R. communis agglutinin since the deduced B chain N-terminal sequence corresponds exactly with that determined for purified R. communis agglutinin B chain over a region where several residue differences occur in the ricin B chain. The nucleotide and deduced amino acid sequences of the R. communis agglutinin precursor are compared with those of the ricin precursor.

L16 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1985:401514 HCAPLUS
DOCUMENT NUMBER: 103:1514

TITLE: Cloning and sequencing of the gene encoding the spike protein of the coronavirus IBV

AUTHOR(S): Binns, Matthew M.; Boursnell, Michael E. G.; Cavanagh, David; **Pappin, Darryl J. C.**; Brown, T. David K.

CORPORATE SOURCE: Houghton Poultry Res. Stn., Houghton/Huntingdon/Cambs., PE17 2DA, UK

SOURCE: Journal of General Virology (**1985**), 66(4), 719-26
CODEN: JGVIAY; ISSN: 0022-1317

DOCUMENT TYPE: Journal

LANGUAGE: English

AB DNA complementary to RNA sequences that encode the surface projection (spike) of the coronavirus infectious bronchitis virus (IBV), strain Beaudette, were cloned into pBR322 by using cDNA primed with a specific oligonucleotide. A 5.3 kilobase viral insert in the clone pMB179 was identified. The region of this clone containing the spike gene was sequenced by the chain termination method, and the gene sequence is presented. The sequence of the primary translation product, as deduced from the DNA sequence, is a polypeptide of 1162 amino acids with a mol. weight of 127,006. The polypeptide is subsequently cleaved to S1 and S2, and partial amino acid **anal.** of the N-terminus of the S1 polypeptide was used to locate the position of this terminus of S1 within the large open reading frame. The amino acid **anal.** also shows an 18-amino acid putative signal sequence on the primary translation product which is not present on the mature S1 polypeptide.

=> => fil beil
FILE 'BEILSTEIN' ENTERED AT 10:35:47 ON 10 MAR 2006

FILE LAST UPDATED ON JANUARY 17, 2006

FILE COVERS 1771 TO 2005.
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L1                STR
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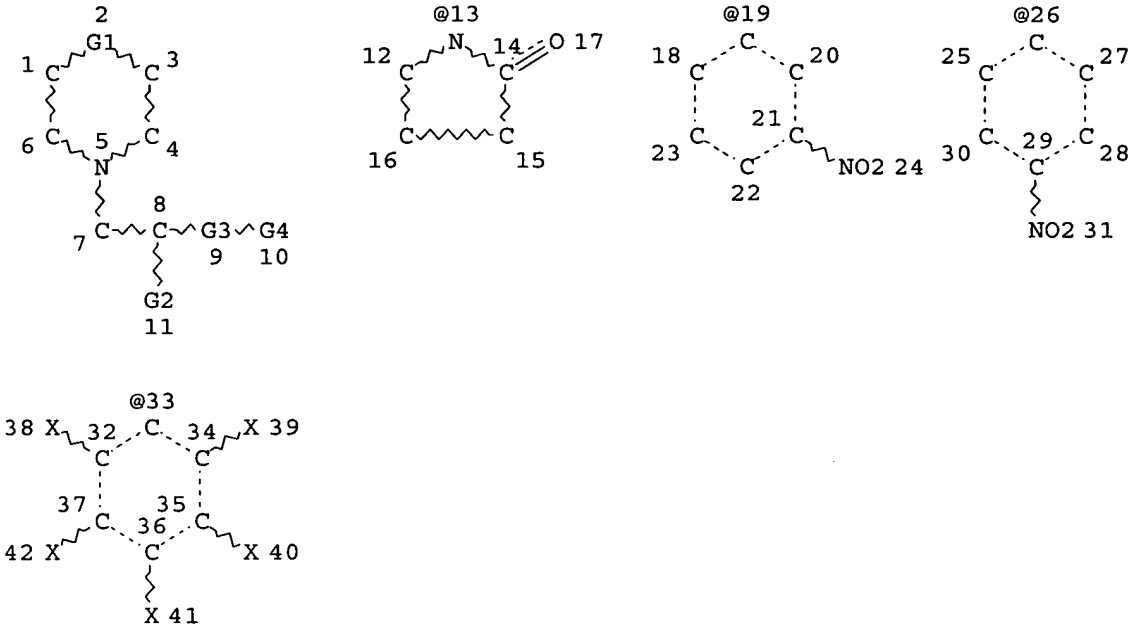


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VAR G3=O/S
VAR G4=13/19/26/33
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  42

STEREO ATTRIBUTES: NONE
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L6               STR
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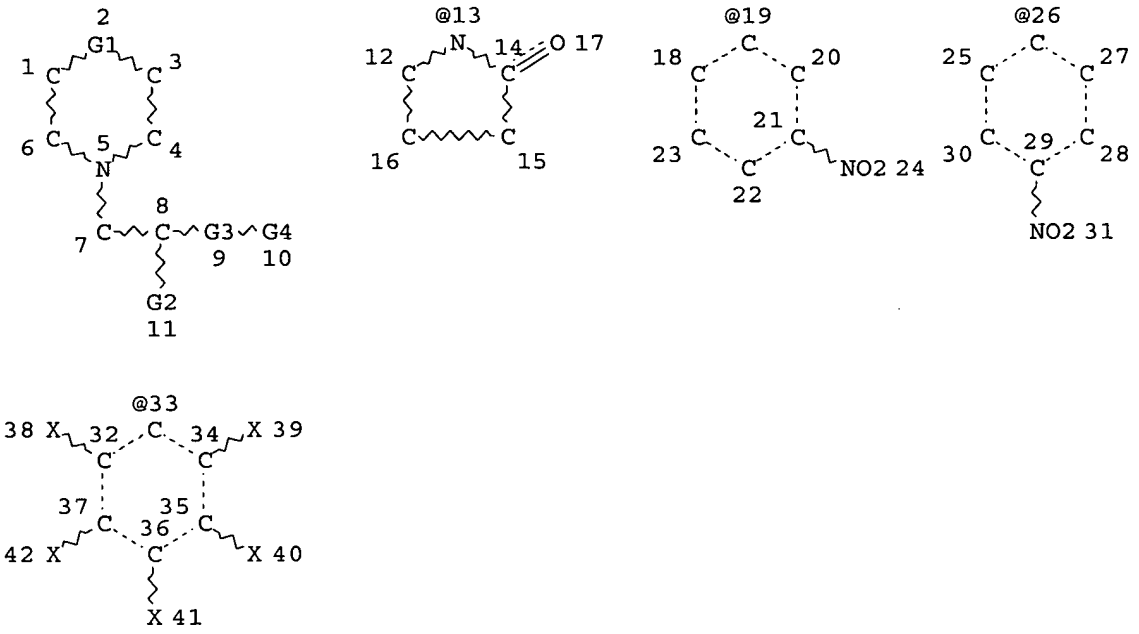

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VAR G2=O/S/N
VAR G3=O/S
VAR G4=13/19/26/33
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 42

STEREO ATTRIBUTES: NONE
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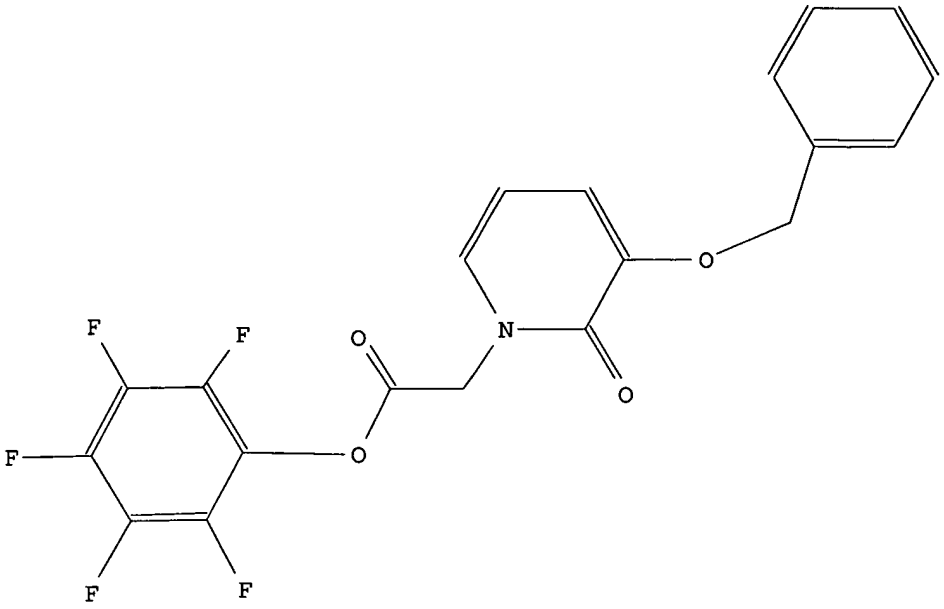
L17 7 SEA FILE=BEILSTEIN SSS FUL L6
L18 6 SEA FILE=BEILSTEIN ABB=ON PLU=ON L17 NOT L7

=> => d cn brn mf fw str rx 1-6

L18 ANSWER 1 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

✓ Chemical Name (CN): (3-benzyloxy-2-oxo-2H-pyridin-1-yl)-acetic acid pentafluorophenyl ester
Autonom Name (AUN): (3-benzyloxy-2-oxo-2H-pyridin-1-yl)-acetic acid pentafluorophenyl ester
Beilstein Records (BRN): 9666299
Molecular Formula (MF): C20 H12 F5 N O4
Molecular Weight (MW): 425.31



Reaction:
RX

Reaction ID (.ID):	9520825
Reactant BRN (.RBRN):	3617212, 2003848
Reactant (.RCT):	(3-benzyloxy-2-oxo-2H-pyridin-1-yl)-acetic acid, pentafluorophenyl trifluoroacetate
Product BRN (.PBRN):	9666299
Product (.PRO):	(3-benzyloxy-2-oxo-2H-pyridin-1-yl)-acetic acid pentafluorophenyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	9520825.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	3.28 g (BRN=9666299)
Reagent (.RGT):	pyridine
Solvent (.SOL):	dimethylformamide
Time (.TIM):	1 hour(s)
Temperature (.T):	20 Cel

Reference(s):

1. Formica, Mauro; Fusi, Vieri; Giorgi, Luca; Guerri, Annalisa; Lucarini, Simone; Micheloni, Mauro; Paoli, Paola; Pontellini, Roberto; Rossi, Patrizia; Tarzia, Giorgio; Zappia, Giovanni, New J. Chem., CODEN: NJCHE5, 27(11), <2003>, 1575 - 1583; BABS-6432739

Reaction:
RX

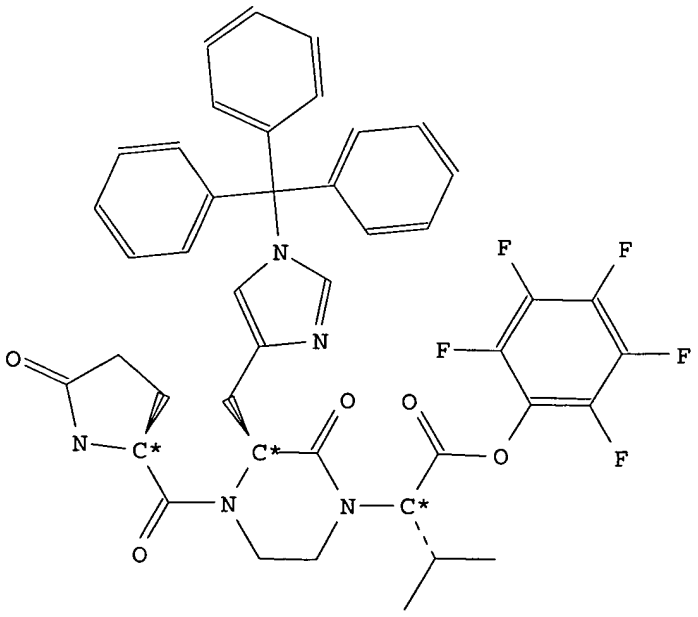
Reaction ID (.ID):	9526447
Reactant BRN (.RBRN):	9666299, 3588279
Reactant (.RCT):	(3-benzyloxy-2-oxo-2H-pyridin-1-yl)-acetic acid pentafluorophenyl ester, 1,7-dimethyl-1,4,7,10-tetraazacyclododecane

Product BRN (.PBRN): 9680624
Product (.PRO): 4-(N), 10-(N)-bis<2-(3-benzyloxy-2-oxo-2H-pyridin-1-yl)acetamido>-1,7-dimethyl-1,4,7,10-tetraazacyclododecane
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 9526447.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 87 percent (BRN=9680624)
Reagent (.RGT): i-Pr2EtN
Solvent (.SOL): dimethylformamide
Time (.TIM): 12 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Formica, Mauro; Fusi, Vieri; Giorgi, Luca; Guerri, Annalisa; Lucarini, Simone; Micheloni, Mauro; Paoli, Paola; Pontellini, Roberto; Rossi, Patrizia; Tarzia, Giorgio; Zappia, Giovanni, New J. Chem., CODEN: NJCHE5, 27(11), <2003>, 1575 - 1583; BABS-6432739

L18 ANSWER 2 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Chemical Name (CN): 3-methyl-2-<2-oxo-4-(5-oxo-pyrrolidine-2-carbonyl)-3-(1-trityl-1H-imidazol-4-ylmethyl)-piperazin-1-yl>-butyric acid pentafluorophenyl ester
Autonom Name (AUN): 3-methyl-2-<2-oxo-4-(5-oxo-pyrrolidine-2-carbonyl)-3-(1-trityl-1H-imidazol-4-ylmethyl)-piperazin-1-yl>-butyric acid pentafluorophenyl ester
Beilstein Records (BRN): 8605792
Molecular Formula (MF): C43 H38 F5 N5 O5
Molecular Weight (MW): 799.80



Reaction:
RX

Reaction ID (.ID):	8555989
Reactant BRN (.RBRN):	8601073, 1912584
Reactant (.RCT):	3-methyl-2-<2-oxo-4-(5-oxo-pyrrolidine-2-carbonyl)-3-(1-trityl-1H-imidazol-4-ylmethyl)-piperazin-1-yl>-butyric acid, pentafluorophenol
Product BRN (.PBRN):	8605792
Product (.PRO):	3-methyl-2-<2-oxo-4-(5-oxo-pyrrolidine-2-carbonyl)-3-(1-trityl-1H-imidazol-4-ylmethyl)-piperazin-1-yl>-butyric acid pentafluorophenyl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8555989.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	DCC, DMAP, Et3N
Solvent (.SOL):	CH2Cl2
Temperature (.T):	0 - 20 Cel
Reaction Type (.TYP):	Esterification

Reference(s):
1. Bhatt, Ulhas; Just, George, Helv.Chim.Acta, CODEN: HCACAV, 83(4), <2000>, 722 - 727; BABS-6234236

Reaction:
RX

Reaction ID (.ID):	8602240
Reactant BRN (.RBRN):	8605792
Reactant (.RCT):	3-methyl-2-<2-oxo-4-(5-oxo-pyrrolidine-2-carbonyl)-3-(1-trityl-1H-imidazol-4-ylmethyl)-piperazin-1-yl>-butyric acid pentafluorophenyl ester
Product BRN (.PBRN):	8600633
Product (.PRO):	3-methyl-2-(2-oxo-4-<(5-oxopyrrolidin-2-yl)carbonyl>-3-<<1-(triphenylmethyl)-1H-imidazol-4-yl>methyl>piperazin-1-yl)butanamide
No. of React. Details (.NVAR):	1

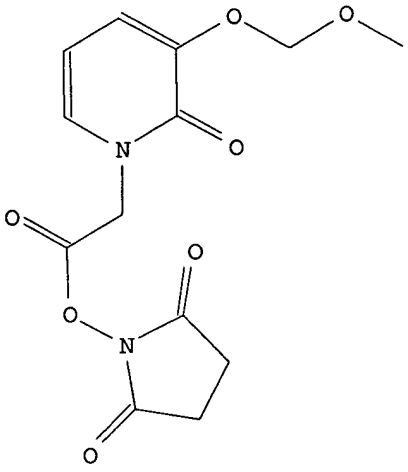
Reaction Details:
RX

Reaction RID (.RID):	8602240.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	6.2 mg (BRN=8600633)
Reagent (.RGT):	NH3
Solvent (.SOL):	ethanol
Time (.TIM):	8 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Substitution

Reference(s):
1. Bhatt, Ulhas; Just, George, Helv.Chim.Acta, CODEN: HCACAV, 83(4), <2000>, 722 - 727; BABS-6234236

L18 ANSWER 3 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Autonom Name (AUN):	(3-methoxymethoxy-2-oxo-2H-pyridin-1-yl)-acetic acid 2,5-dioxo-pyrrolidin-1-yl ester
Beilstein Records (BRN):	8217191
Molecular Formula (MF):	C13 H14 N2 O7
Molecular Weight (MW):	310.26



Reaction:
RX

Reaction ID (.ID):	5086550
Reactant BRN (.RBRN):	8202407, 113913
Reactant (.RCT):	(3-methoxymethoxy-2-oxo-2H-pyridin-1-yl)-acetic acid, N-hydroxy-succinimide
Product BRN (.PBRN):	8217191
Product (.PRO):	(3-methoxymethoxy-2-oxo-2H-pyridin-1-yl)-acetic acid 2,5-dioxo-pyrrolidin-1-yl ester
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	5086550.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	22 percent (BRN=8217191)
Reagent (.RGT):	dicyclohexylcarbodiimide

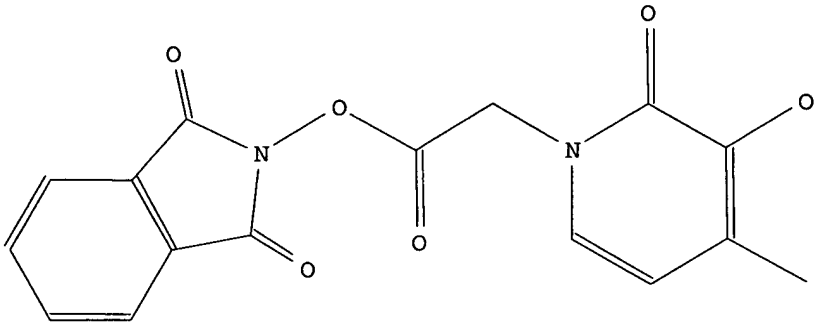
Reference(s):

1. Rai, Bijaya L.; Khodr, Hicham; Hider, Robert C., Tetrahedron, CODEN: TETRAB, 55(4), <1999>, 1129 - 1142; BABS-6157581

L18 ANSWER 4 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Chemical Name (CN):	(3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester
Autonom Name (AUN):	(3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester

Beilstein Records (BRN): 7944429
Molecular Formula (MF): C16 H12 N2 O6
Molecular Weight (MW): 328.28



Reaction:
RX
Reaction ID (.ID): 4862410
Reactant BRN (.RBRN): 7920668, 131208
Reactant (.RCT): (3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetic acid, N-hydroxy-phthalimide
Product BRN (.PBRN): 7944429
Product (.PRO): (3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4862410.1
Reaction Classification (.CL): Preparation
Reagent (.RGT): dicyclohexylcarbodiimide
Solvent (.SOL): tetrahydrofuran
Other Conditions (.COND): 0 deg C, 20 min; room temperature, 1 h
Reference(s):
1. Fox, Raymond C.; Taylor, Paul D., Synth.Commun., CODEN: SYNCAV, 28(9), <1998>, 1563-1574; BABS-6089572

Reaction:
RX
Reaction ID (.ID): 4866678
Reactant BRN (.RBRN): 7944429, 1739626
Reactant (.RCT): (3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester, tris-(2-amino-ethyl)-amine
Product BRN (.PBRN): 7964315
Product (.PRO): N-<2-(bis-<2-<2-(3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetylamino>-ethyl>-amino)-ethyl>-2-(3-hydroxy-4-methyl-2-oxo-2H-pyridin-1-yl)-acetamide
No. of React. Details (.NVAR): 1

Reaction Details:

RX

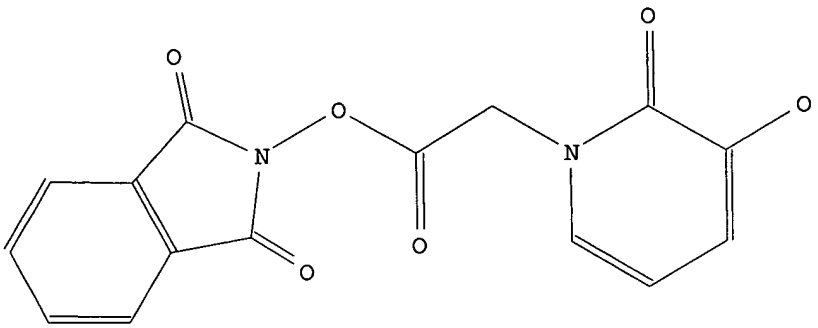
Reaction RID (.RID):	4866678.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	40 percent (BRN=7964315)
Reagent (.RGT):	Et3N
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	1 hour(s)
Other Conditions (.COND):	Ambient temperature

Reference(s):

1. Fox, Raymond C.; Taylor, Paul D., Synth.Commun., CODEN: SYNCAV, 28(9), <1998>, 1563-1574; BABS-6089572

L18 ANSWER 5 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Chemical Name (CN):	(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester
Autonom Name (AUN):	(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester
Beilstein Records (BRN):	7944361
Molecular Formula (MF):	C15 H10 N2 O6
Molecular Weight (MW):	314.25



Reaction:

RX

Reaction ID (.ID):	4862403
Reactant BRN (.RBRN):	1453406, 131208
Reactant (.RCT):	(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetic acid, N-hydroxy-phthalimide
Product BRN (.PBRN):	7944361
Product (.PRO):	(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester
No. of React. Details (.NVAR):	1

Reaction Details:

RX

Reaction RID (.RID):	4862403.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	dicyclohexylcarbodiimide
Solvent (.SOL):	tetrahydrofuran
Other Conditions (.COND):	0 deg C, 20 min; room temperature, 1 h

Reference(s):
1. Fox, Raymond C.; Taylor, Paul D., Synth.Commun., CODEN: SYNCAV, 28(9), <1998>, 1563-1574; BABS-6089572

Reaction:
RX

Reaction ID (.ID):	4866677
Reactant BRN (.RBRN):	7944361, 1739626
Reactant (.RCT):	(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetic acid 1,3-dioxo-1,3-dihydro-isoindol-2-yl ester, tris-(2-amino-ethyl)-amine
Product BRN (.PBRN):	3643079
Product (.PRO):	N-<2-(bis-<2-<2-(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetylamino>-ethyl>-amino)-ethyl>-2-(3-hydroxy-2-oxo-2H-pyridin-1-yl)-acetamide
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	4866677.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	33 percent (BRN=3643079)
Reagent (.RGT):	Et3N
Solvent (.SOL):	tetrahydrofuran
Time (.TIM):	1 hour(s)
Other Conditions (.COND):	Ambient temperature

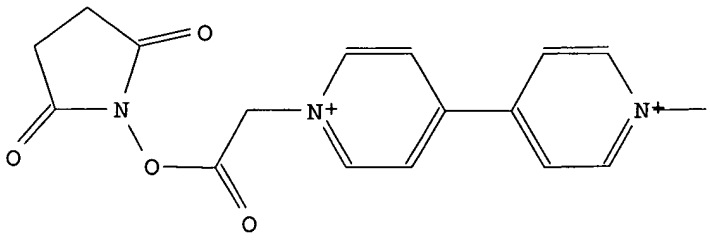
Reference(s):
1. Fox, Raymond C.; Taylor, Paul D., Synth.Commun., CODEN: SYNCAV, 28(9), <1998>, 1563-1574; BABS-6089572

L18 ANSWER 6 OF 6 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Chemical Name (CN):	succinimide ester of 1-methyl-1'-carboxymethyl-4,4'-bipyridinium perchlorate
Beilstein Records (BRN):	5846197
Molecular Formula (MF):	C17 H17 N3 O4 . 2 Cl O4
Molecular Weight (MW):	327.34, 99.45

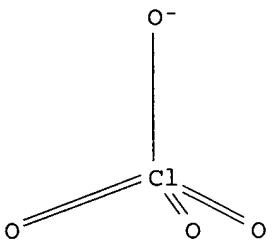
CM 1

FBRN 5832906
FMF C17 H17 N3 O4



CM 2

FBRN 3587878
FMF Cl O4



Reaction:
RX

Reaction ID (.ID):	1645997
Reactant BRN (.RBRN):	5844862, 113913
Reactant (.RCT):	1-methyl-1'-carboxymethyl-4,4'-bipyridinium perchlorate, N-hydroxy-succinimide
Product BRN (.PBRN):	5846197
Product (.PRO):	succinimide ester of 1-methyl-1'-carboxymethyl-4,4'-bipyridinium perchlorate
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	1645997.1
Reaction Classification (.CL):	Preparation
Reagent (.RGT):	1,3-dicyclohexylcarbodiimide (DCC)
Solvent (.SOL):	acetonitrile
Time (.TIM):	16 hour(s)
Temperature (.T):	-5 - 20 Cel

Reference(s):
1. Tsukahara, Keiichi; Todorobaru, Hiromi, Chem.Lett., CODEN: CMLTAG(7), <1992>, 1181-1184; BABS-5704527

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